Investigating the neutral sodium emissions observed at comets

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THESIS

Submitted for the degree of
Doctor of Philosophy, University College London

2017
I, Kimberley Siân Birkett, confirm that the work presented in this thesis is my own. Where information has been derived from other sources, I confirm that this has been indicated in the thesis.
Neutral sodium emission is typically very easy to detect in comets, and has been seen to form a distinct neutral sodium tail at some comets. If the source of neutral cometary sodium could be determined, it would shed light on the composition of the comet, therefore allowing deeper understanding of the conditions present in the early solar system. Detection of neutral sodium emission at other solar system objects has also been used to infer chemical and physical processes that are difficult to measure directly.

Neutral cometary sodium tails were first studied in depth at comet Hale-Bopp, but to date the source of neutral sodium in comets has not been determined. Many authors considered that orbital motion may be a significant factor in conclusively identifying the source of neutral sodium, so in this work details of the development of the first fully heliocentric distance and velocity dependent orbital model, known as COMPASS, are presented. COMPASS is then applied to a range of neutral sodium observations, including spectroscopic measurements at comet Hale-Bopp, wide field images of comet Hale-Bopp, and SOHO/LASCO observations of neutral sodium tails at near-Sun comets.

The author finds that COMPASS is relatively successful at reproducing the morphology of the neutral sodium tails seen in wide field images, and to a lesser extent the intensity profiles produced by spectroscopic measurements. The success of COMPASS indicates that the current understanding of the physics of the production and evolution of neutral cometary sodium is broadly accurate. Using a simplistic Finson and Probstein [1968] dust tail source the author also finds that a source of neutral sodium within the dust tail is likely to result in a secondary neutral sodium tail feature, that has not yet been observed to the best of their knowledge.
Acknowledgments

The work in this thesis was supported by STFC grant ST/K50239X/1. Thanks to UCL Graduate school and Federation of Finnish Learned Societies Grant for support to attend ACM in July 2014, and to the Royal Astronomical Society for support to attend AGU in December 2013.

I would like to thank my supervisors, Geraint Jones and Andrew Coates, for their support and guidance throughout my PhD. Thanks to the near-Sun comets team at ISSI, particularly Colin Snodgrass. Special thanks to Karl Battams for helping me make sense of Solarsoft and to Lin Gilbert, my IDL guru.

Thanks also to the Planetary and Plasma groups at MSSL - particularly Yudish and the guys from 108 - and to cake club and croquet for making long afternoons seem shorter.

Finally, thank you to my family: Mum (Margi), Dad (Ian), Luke, Grandma (Terry), Grandad (Jim), Muriel and Anthony for their patience, understanding and support.
“I may not have gone where I intended to go, but I think I have ended up where I needed to be.” Douglas Adams, The Long Dark Tea-Time of the Soul.
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Chapter 1

Introduction

This chapter discusses the basic principles relevant to the study of cometary sodium presented in this thesis. A brief outline of the current level of understanding of cometary science is presented and why the understanding of the cometary environment, particularly the study of neutral sodium observed in comets, may be important to the study of Solar System formation and space physics more generally is discussed.

1.1 Why Study Comets?

Comets are remnants of Solar System formation and therefore represent the best objects to study to allow insight into its evolution. The inner regions of cometary nuclei remain largely unaffected by the Solar System environment, as incident solar radiation and cosmic rays are only thought to penetrate their outer layers. Cometary nuclei therefore contain the least processed material in the Solar System, potentially pre-solar grains [Brandt and Chapman, 1992; Glassmeier et al., 2007]. The dust particles detected at comets also seem to contain a high percentage of refractory organic \textit{CHON} material, which may have deposited the material required for life on Earth [Huebner, 1990]. Studying cometary science is therefore important to furthering our understanding of our Solar System.

Comets may also be the source Earth’s vast quantities of water and may shed light onto how the Solar System formed and how planets like the Earth may contain significant amounts of water despite being relatively close to the Sun [Izidoro et al., 2013].

Studying the cometary environment also provides a unique test of our current understanding of the plasma interactions and physical/chemical processes occurring within the Solar System. Understanding these mechanisms has implications for many other fields within space physics, such as improving the understanding of space weather and planetary interactions with the solar wind.
In summary there are three principal reasons to study cometary science:

1. Comets are remnants of Solar System formation.

2. Comets may be a significant source of water on Earth.

3. The cometary environment represents a unique challenge to our current understanding of Space Physics and Planetary Science.

For the remainder of this chapter we discuss the background of comet nucleus theory, comet tail formation and the origin of comets. Good reviews of these topics are available in Huebner [1990], Fernandez and Jockers [1983] and Fernandez [2005].

1.1.1 What is a comet?

A comet is a celestial body composed of a mixture of volatile and non-volatile material. The core of the comet, known as the nucleus, is typically a few kilometres in size. Initially a sand bank model was proposed by Lyttleton [1948] to understand the structure of the core of a comet. In this model the nucleus is pictured as a weakly gravitationally bound collection of dust grains of various sizes with adsorbed volatile material on their surfaces. Adsorption allowed volatile material to be trapped on the surface of the dust grains by surface forces and gradually released as the comet approached the Sun and the collisions between dust grains increased. However, the sand bank comet nucleus model could not satisfactorily explain how a comet could be observed to survive a close perihelion passage or why gas densities much higher than predicted were observed (notably in the ultraviolet emissions indicative of the Lyman alpha electronic transitions observed by Keller [1976]).

Whipple [1950] proposed the icy conglomerate model for the comet nucleus, which forms the basis of our current understanding of cometary nuclei. In the icy conglomerate model, comet nuclei are described as a solid, inhomogeneous mixture of frozen volatile ices and non-volatile dust. As the icy conglomerate comet nucleus approaches the Sun the outer layers of icy material begin to sublimate due to solar visible and ultraviolet radiation, releasing dust trapped within the ice. The sublimating surface ice would leave a residue of dusty material, known as the mantle, and a trapped core composed of a mixture of dust and volatiles. Comets lose one metre of material from their surfaces per perihelion passage on average [Meech et al., 2015].

As a cometary nucleus is so small (and of very low mass) the sublimated particles would be essentially gravitationally unbound and the resulting cloud of gas and dust would form an extended cometary coma. The gravitationally unbound atmosphere is a key feature of the cometary environment, distinguishing its interactions from those of other Solar System bodies.

In the icy conglomerate model, solar radiation could not penetrate deeply beneath the
surface of the nucleus. Therefore volatile material that was located deep beneath the surface of the nucleus would not sublimate until it had been exposed by the removal of surface material via sublimation. The icy conglomerate model was therefore successful in explaining why the innermost regions of the comet remained intact following multiple perihelion passages. It also successfully explained Whipple’s observations of non gravitational forces acting on comet 2P/Encke [Whipple, 1950]. Ice sublimating on the sunward side of a comet nucleus would result in a rocket effect that would give the nucleus a net acceleration away from the Sun.

A diagram of the potential structure of the surface layers of the comet nucleus based on this theoretical description is given in figure 1.1. It highlights the complexity of the processes involved in releasing material from cometary nuclei, particularly as different volatiles (H$_2$O, CO, CO$_2$ etc) have different sublimation temperatures and therefore sublimation of different volatiles occurs at different depths beneath the mantle.

Figure 1.1: Diagram illustrating the theoretical surface structure of a cometary nucleus. Reproduced from Bleeker et al. [2001], which was adapted from Rickman [1991].

The dramatic coma and tail features observed at comets are a direct result of the interaction of the bare comet nucleus with the solar wind and solar radiation. Some solar radiation incident on the nucleus would be reflected, but a sufficient amount may be absorbed that the outer layers of the nucleus may begin to sublimate. Far from the Sun, when a comet is of relatively low activity and has no significant coma, the solar wind ions may directly impact the surface of the comet nucleus and release sputtered material. Direct sputtering of the refractory elements Na, K, Si, and Ca, has recently been observed by the Rosetta mission to comet 67P/Churyumov-Gerasimenko [Wurz et al., 2015]. However, as the activity of the comet increases the sublimating material would form a distinct coma. During these conditions, direct interaction between the solar wind and the comet nucleus is impossible, although solar radiation may still penetrate to the nucleus and sublimate material as the coma is optically thin [Fernandez, 1999]. Solar extreme ultraviolet radiation can then charge some of the neutral gas within the coma, causing it to become ionised and constitute an obstacle to the solar
Why Study Comets?

wind flow. The interaction between the charged coma and the solar wind is discussed in more detail in chapter 1.1.3.

1.1.2 Origin and Formation of Comets

In this chapter we present the most plausible explanation to date of the existence of comets, which provides some insight into their structure and characteristics. An alternative taxonomy of comets that may be more appropriate than the broad discussion of long/short period groups discussed here is given in Appendix A. A discussion of the orbital parameters used to classify comets is also presented in Appendix A. As comets are considered to be the key observable remnants of Solar System formation, understanding of the formation of comets is inexorably linked to our understanding of the formation of the Solar System. Many details surrounding the formation of the Solar System remain elusive, but the theory presented here is widely accepted.

Alternative theories to those presented in the paragraphs that follow, for example those of [Lyttleton, 1951, 1948] that suggest that comets are interstellar objects that are captured by the gravitational pull of the larger planets and the Sun, have not been successful at explaining the orbital characteristics of observed comets. If comets were truly of interstellar origin, we would expect the distribution of cometary orbits to be random, many observed comets to have hyperbolic orbits and a concentration of perihelia near the Galactic plane. In reality the distribution of long period cometary orbital parameters is concentrated around \((1/a)_{\text{orig}} \approx 10^{-5}\), most comets do not have hyperbolic orbits and there is no concentration of perihelia near the Galactic plane [Oort, 1950; Guliyev and Dadashov, 2010]. These observations support a source of comets within the Solar System resulting from its formation.

The Solar System began as a condensation of a dense region of the interstellar medium. Possessing a non-zero initial angular momentum, this would have condensed into a compacted central nucleus. This central nucleus formed the precursor to our Sun, and around it, smaller planetesimal objects would have condensed that eventually formed the planets. However a large fraction these planetesimals would not have had suitable orbits to take part in the formation of the planets, and instead would have been subjected to large perturbations of their orbits as the planets formed and the gravitational forces shifted within the newly forming Solar System. The mass of a comet is typically less than \(10^{-10}\) times the mass of the Earth [Huebner, 1990]. Therefore the orbits of comets may be perturbed by the presence of a planet, but the effect of a comet on the orbit of a planet is negligible.

The orbits of these objects would have diffused outwards due to these planetary perturbations, resulting in many of them being ejected from the Solar System. The remaining planetesimals would have continued to diffuse outwards and at a sufficient distance from the planets, perturbations to the orbits of these objects due to planetary gravitational
forces would have become relatively weak, and perturbations due to tidal forces within the galaxy and gravitational attractions from other stars would begin to dominate.

The planetary gravitational forces exerted upon the planetesimals would have allowed them to change the major axes of their orbits but, due to the initial angular momentum of the interplanetary medium from which they condensed, would have caused them to remain primarily in the ecliptic plane. However, perturbations due to other stars and galactic tidal forces could have acted in any direction, resulting in a range of orbital parameters for these objects. For objects at this distance, in a region extending from roughly $1.7 \times 10^4$ AU to $1 \times 10^5$ AU [Huebner, 1990], planetary perturbations to their orbits are negligible and would only very rarely be perturbed by stellar motions or galactic tidal forces. Therefore objects in this region, known today as the Oort cloud, would have been largely stable [Oort, 1950], providing a suitable source of the long period comets. Oort [1950] initially proposed this reservoir of comets after noting a concentration of long period comets with $(1/a)_{\text{orig}} \approx 10^{-5}$.

Once the orbits of objects within the Oort cloud were perturbed by the motion of passing stars and caused to travel into the inner Solar System, many could be potentially affected by Jupiter’s strong gravitational force. Through perturbations to their orbits inactive comets at the edge of the Solar System are brought into the inner Solar System (some to within a few solar radii of the Sun) therefore allowing study of these otherwise unobservable bodies.

Cosmic rays and nuclear radiation are the dominant source of radiation for a comet at the outer edges of the Solar System [Bleeker et al., 2001]. Fundamental changes in the outer layers of the comet nucleus may have occurred due to irradiation from cosmic rays whilst the comet was in its initial reservoir (i.e. Oort cloud or scattered disk), however it is likely that these outer layers are lost on the comet’s first passage into the inner Solar System. Interstellar cosmic radiation may also cause dynamically new comets (see Appendix A for more details) to display enhanced activity on their first passage into the inner Solar System, as it may result in volatile material becoming trapped within the crust layer [Huebner, 1990]. If nuclear activity is significant within the core of a comet nucleus whilst it is in the outer edges of the Solar System, an increase in core temperature would result. Such an increase in temperature may lead to diffusion of volatiles within the core and may also be capable of changing material in the interior of the nucleus [Wallis, 1980].

There must exist a source of short period comets in the outer edges of the Solar System, because following their multiple trips around the Sun these bodies would have been reduced to insignificant quantities of mass over the current age of the Solar System (approximately 4.5 billion years [Bochsler, 2000]) and would therefore no longer be observable. Short period comets typically have inclinations of less than $30 - 35^\circ$ [Weissman and Campins, 1993; Stern, 2003] and are therefore considered to have originated in regions other than the Oort cloud (where a range of inclinations is present).
Today we know these regions as the Kuiper Belt and Scattered Disk. The Oort Cloud, Kuiper Belt and Scattered Disk (shown in figure 1.2) formed from the same protoplanetary disk, but it is likely that they originated in different regions. The Scattered Disk is a region located at the edge of the Kuiper Belt, characterised by objects scattered to a much wider range of inclinations than is present in the Kuiper Belt. The orbits of objects currently within the Kuiper Belt/Scattered Disk were such that as they were diffusing outwards their orbits were perturbed by the gravitational field of Neptune and Jupiter/Neptune respectively, effectively preventing them from escaping into the Oort cloud [Duncan, 1997].

![Figure 1.2: Diagram illustrating positions of the comet reservoirs on the outer edges of the Solar System. Reproduced from Stern [2003].](image)

1.1.3 Key features of the cometary environment

The icy conglomerate model proposed by Whipple [1950] is the most successful to date at explaining cometary observations and provided the basis for which the theory of the structure of the comet nucleus was to be developed (see chapter 1.1.1). As the comet nucleus is so small, observations of comets typically focus on their most clearly distinguishable features: the coma, the ion tail (and related plasma boundaries detected in situ) and the dust tail. Comet tails are typically significantly larger than the coma, and therefore easier to observe, for most active comets. In this chapter we discuss each of these aspects of the cometary environment briefly, ending with a discussion of the neutral comet tails studied in this thesis.
Coma In a comet where activity is just commencing, the cometary tails that were the key features observable before the era of telescopes have not yet formed. Instead, the dominant feature will be the cometary coma.

A typical comet nucleus is covered in an inactive mantle layer (for comets that are not dynamically new, caused by deposition of refractory material following a period of activity) or a crust layer (for dynamically new comets, caused by cosmic ray treatment) and does not have a uniform composition or shape, based on in situ observations from the comet Halley armada of spacecraft and subsequent missions [Huebner, 1990]. The nucleus is the primary source for all material observed in the coma, but the nonuniformity of the nucleus also means that it does not emit material isotropically.

Initial theories suggested that dust, which had been released by sublimating nuclear volatiles, was predominantly ejected in the sunward direction on the sunward side of the comet and subsequently predominantly pushed in an antisunward direction by solar radiation pressure, ‘behaving like a fountain that ejects its water upwards’, as described by Huebner [1990]. More modern theories, supported by measurements such as those taken by the Rosetta mission to comet 67P/Churyumov-Gerasimenko (an example is shown in figure 1.3), suggest a series of complex surface features and jets, some of which occur on the side of the comet whilst in darkness once the comet had obtained sufficient thermal energy from solar irradiation [Sierks et al., 2015; Thomas et al., 2015]. Jets emanating from the surface of a comet nucleus may result in a wide variety of different structures within the coma (see figure 1.4).

Figure 1.3: Image from the OSIRIS camera taken on 23 September 2014. OSIRIS one of the suite of instruments on board the Rosetta spacecraft, which is currently in orbit around comet 67P/Churyumov-Gerasimenko. Jets from the Hapi region on the surface of the comet, and the non-uniformity of the comet nucleus and active regions are apparent. Reproduced from Sierks et al. [2015].

The cometary coma provides the best current representation of the composition of the cometary nucleus. With the first soft comet landing accomplished by the Philae landing (a key part of the Rosetta mission) in November 2014, it was hoped that the first direct samples of the nucleus could be taken. Philae contained a drill which was to enable
samples to be taken of the surface layers of the nucleus which could then be analysed and compared to the coma analysis, but unfortunately the lander was not positioned correctly due to the failure of some of the systems designed to ensure the lander was suitably anchored on the comet’s surface. The drill on Philae, although successfully deployed, was unable to obtain a sample before the lander ran out of power in the lander’s darkened resting location, which ensured that the solar panels onboard Philae could not recharge at that time. Initial signals from Philae had been received indicating that the lander was still functional in June 2014, but reliable lander communications had not yet been established and although we hope the Philae will power up and recommence operations, it appeared unlikely that the drill would be redeployed before cometary activity was so great that lander operations would become too difficult. The Rosetta mission ended on 30 September 2016 with a controlled impact onto the comet’s surface (see the Rosetta/Philae blog for more details [Various [2015]]. As no further communications from the lander had been received at the end of the mission, to date the best current representation of the composition of the cometary nucleus remains the composition of the coma.

Observations and in situ measurements of the cometary coma have shown that it is primarily composed of $H_2O$. Many other species have also been detected in the coma including $H, C, C_2, C_3, CH, CN, ^{12}C^{13}C, HCN, CH_3CN, NH, NH_2, O, OH, Na, K, Ca, V, Cr, Mn, Fe, Co, Ni, Si, S$ and $Cu$ [Whipple, 1976; Wurz et al., 2015]. Measurements taken from cometary missions have also shown that a large fraction of dust is entrained within the outflowing volatile material [Huebner, 1990].

Figure 1.4: Possible dust structures resulting from a range of observational geometries and different jet positions, reproduced from Sekanina [1987].
**Ion Tail and Plasma Boundaries** Once a sufficient amount of material has been released from a comet nucleus by solar radiation and formed a cometary coma (composed of neutral gas and dust) this material may be ionised by charge exchange with the solar wind and photoionisation by solar radiation. The main cometary species is $H_2O$, which is primarily ionised via photoionisation by solar extreme ultraviolet radiation [Coates and Jones, 2009; Cravens, 2004].

The cometary coma prevents direct interaction between the solar wind and the cometary nucleus, but charged cometary material appears as an obstacle to the interplanetary magnetic field (IMF) that is frozen into the solar wind. At active comets this may lead to the formation of different plasma boundaries that have been detected in situ by missions such as Giotto and Rosetta. A representation of the plasma boundaries detected in situ at comets is shown in figure 1.5. Cometary ion pickup also increases the mass flux within the solar wind. Therefore in order to conserve momentum the solar wind is slowed, resulting in the IMF being draped around the comet and the formation of the characteristic cometary ion tail (a process called ‘mass loading’). The forces acting on the ions within the cometary ion tail are relatively strong, and therefore the ion tail is typically observed as very generally linear. The interactions between cometary constituents, the solar wind and the IMF also leads to the formation of various plasma boundaries, such as the Bow Shock, Contact Surface, Cometopause, Mystery Boundary, Ion Pileup Boundary and Magnetic Pileup Boundary (see Coates [1997]; Coates and Jones [2009] for more information).

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**Figure 1.5:** Plasma boundaries found around an active comet, reproduced from Stoeva et al. [2005].

Plasma processes occur differently at comets that approach within a few solar radii, where all the cometary material (including the usually refractory dust particles) may be sublimated rapidly. In this chaotic case distinct, observable plasma boundaries are unlikely to be formed.
Dust Tail Once sufficient material is released from the nucleus, cometary dust may be observed to form its own distinct tail. Cometary dust reflects the visible solar spectrum, and therefore the cometary dust tail (sometimes known as a type II tail) is typically whiter in colour than the ion tail. In order to scatter light in this way, dust particles must be larger than the wavelength of visible light, and typically individual dust particles are approximately $1 - 10\mu m$ in size [Huebner, 1990]. In comets a range of dust particles and clusters are observed, and these are considered to range in size from nanometres to metres in size. Two distributions of dust particles, one composed of fluffy aggregates and the other of compact particles, have been identified in-situ by Fulle et al. [2015] at comet 67P using GIADA (Grain Impact Analyzer and Dust Accumulator) onboard the Rosetta spacecraft. Fulle et al. [2015] state that the fluffy aggregates constitute a negligible amount of mass loss from the cometary nucleus but have a steeper side distribution than the compact particle distribution, which may account for the difference between the dust size distribution observed in situ [Rotundi et al., 2015] and that observed from remote sensing on Earth [Fulle et al., 2010].

A cometary dust tail may form when a significant amount of non-volatile material is entrained within the outflow of sublimating gas from the cometary nucleus. The dust will be produced with a range of sizes, masses and ‘fluffiness’ and will therefore interact with solar radiation differently. Dust particles are typically characterised by their $\beta$ parameter, which was originally introduced by Finson and Probstein [1968] in order to model dust tails and is given by:

$$\beta = \frac{F_{rad}}{F_{grav}}$$

(1.1)

where $F_{rad}$ is the magnitude of the force on the dust particle due to solar radiation pressure (directed away from the Sun) and $F_{grav}$ is the magnitude of the gravitational force on the dust particle due to the mass of the Sun (directed towards the Sun). The orbits of particles with the same $\beta$ will follow the same dynamics. These paths are known as syndynes. Typically the heaviest dust, for which $F_{grav}$ dominates, will therefore lie along the trajectory of the comet’s orbit. The orbits of particles with different $\beta$ values but that are released from the comet nucleus at the same time are known as synchrones. The curved mesh of synchrones over a suitable age of observable dust and syndynes of suitable $\beta$ values for a particular comet will therefore map out the cometary dust tail, and explains why the dust tail is typically curved and broader than the ion tail. This approach has been particularly successful in modelling outbursts at comets. We use a similar approach in chapter 8.

Comet dust is not considered to change significantly over the lifetime of the comet as it is not likely to sublimate (except for the very extreme case where comets approach within a few solar radii), but may be modified slightly by solar wind sputtering (see chapter 1.1.1). Interplanetary dust particles are considered by Schramm et al. [1989]
to have their origin in asteroidal and cometary material, and these typically consist of refractory silicates and carbonaceous material.

**Neutral Tails** Neutral atom emissions have been observed in the spectra of many comets and identified as potential indicators of chemical processes occurring in cometary coma, as they are usually dissociation products [Cremonese et al., 2002]. Table 1.1 gives some examples of neutral elements typically observed in cometary comae.

The $g$ factor, or fluorescence rate (in $\text{photons s}^{-1}\text{atom}^{-1}$), characterises the atomic efficiency of a resonant scattering process [Combi et al., 1997; Kawakita and Fujii, 1998] (see chapter 2.2 for more information). Lithium has a high $g$ factor but its abundance is relatively low, whereas sulphur has a relatively high abundance but a small $g$ factor. Oxygen is typically much more abundant than sodium in comets but the $g$ factor is $10^6$ times smaller than that of sodium and it is very difficult to obtain wide field images in the ultraviolet (the typical wavelength listed in tables is in the ultraviolet). Oxygen also emits in the visible, but in this range the strong telluric emission interferes [Cremonese et al., 2002]. Potassium has been observed in comets but as the abundance and $g$ factor are not as high as sodium, it is much more difficult to obtain a high enough signal to noise ratio in a particular image to be able to observe a well defined neutral potassium tail.

Therefore in reality, although it is potentially possible to measure many other neutral elements in cometary comae, only neutral sodium atom emission can be detected at large distances from the comet nucleus. This is primarily due to the sodium atom’s extremely high efficiency in the resonant scattering of solar radiation making the emission detectable, even when the column density is relatively low [Cremonese et al., 1997b].

![Removed due to copyright.](image)

**Table 1.1: Table showing chemical parameters for unshifted absorption lines at 1 AU for some key neutral atoms, reproduced from Cremonese et al. [2002] (values collected from Chamberlain and Hunten [1987]; Sprague et al. [1995, 1996]; Hunten and Sprague [1997]). Solar abundances listed are relative to Si. $\lambda$ is the usual wavelength observed for the relevant species. See chapter 2.2 for a discussion of the relevance of the $g$ factor.**

A distinct tail composed of neutral atoms was first studied in some detail with the observation of a neutral sodium tail at comet Hale-Bopp (C/1995 O1) in 1997 [Cremonese et al., 1997b]. The formation of the neutral sodium tail is complex (see chapter 2.2), but it is the high absorption and emission efficiency of the sodium D transition that ensures
that sodium is readily observable in comets even when the column density is low. The most observed neutral sodium tail to date is undoubtedly that of comet Hale-Bopp, but other comets have also displayed this feature, as presented in this thesis.

Other neutral cometary tails, composed of species other than sodium, have been speculated. When an apparently neutral cometary tail was observed by the STEREO-A spacecraft at comet McNaught (C/2006 P1), Fulle et al. [2007] noted that the band pass of the HI1-A instrument on board STEREO-A spacecraft (see chapter 3) did not contain the wavelength for sodium, and therefore could not image a neutral sodium tail. Fulle et al. [2007] suggested that the feature they observed was instead the first imaged neutral iron tail.

1.2 Why Study Cometary Sodium?

Neutral sodium emission was first detected in cometary spectra in 1881 and initially used to estimate the speed of the cometary nucleus, but the source of neutral sodium in comets was unclear [Brandt and Chapman, 2004]. Neutral sodium D line emission is a very bright feature in cometary comae and therefore relatively easy to detect in active comets.

In 1960 Nguyen-Huu-Doan recorded a seven degree sodium tail in comet Mrkos (C/1957 P1) using a Schmidt camera with an objective prism [Nguyen-Huu-Doan, 1960]. The sodium tail was identified but the extended emission was obscured by the continuum of the dust tail.

It was not until 1997 that the morphology of an extended sodium emission, indicative of a third type of cometary tail, was imaged at comet Hale-Bopp (C/1995 O1) by Cremonese et al. [1997b]. This observation triggered an extensive campaign to study the neutral sodium tail of this comet, but despite the extensive observational campaign the source of sodium at comets remains unknown [Cremonese et al., 2002] (see chapter 2 for more details).

Most neutral atoms observed at comets are dissociation products [Cremonese et al., 2002], meaning that they are produced in a reaction whereby the parent molecules split into smaller particles. For example the presence of large abundances of $H$ and $OH$ in the cometary coma in roughly equal quantities provided in the initial evidence for the presence of water, $H_2O$, at comets [Brandt and Chapman, 2004]. $H_2O$ is known to dissociate into $H$, $O$, $OH$ and $H_2$, and therefore studying the large quantities of $H$ and $OH$ gives an insight into the production of water in comets. Similarly, observation of cometary sodium has the potential to allow insight into the mechanisms occurring in comets and into the formation of cometary nuclei [Cremonese, 1999]. Sodium atoms are very efficient in the resonant scattering of solar radiation (see chapter 2.2). Therefore sodium emission is relatively easy to detect even if the column density is low. For
example sodium has been used as a tracer of atmospheric interactions with the plasma torus at Io despite its one percent abundance in Io’s atmosphere [Cremonese et al., 1997b].

Studying cometary sodium could also allow insight into the formation of the cometary nucleus. Cosmic rays and nuclear radiation from nucleotides within the nucleus are the dominant sources of heating of a comet nucleus whilst it is in the outer edges of the Solar System and Wallis [1980] suggest that, if present in sufficient quantities, the radioactive nucleotide, $^{26}$Al could produce enough heating within the core of the comet nucleus to result in melting of snow and dust balls in its interior if the comet is larger than $3 - 6$ km in radius.

Recent modelling results from Ellinger et al. [2015] show that sodium would have initially been trapped in rocks in the protosolar nebula and proposes that radiogenic heating (such as that described by Merk and Prihnik [2006], Irvine et al. [1980] and Wallis [1980]) could have resulted in liquid water in the cores of comet nuclei whilst on the outer edges of the Solar System. If liquid cores once existed in cometary nuclei, then the sodium present within rocky cometary material would have effectively been washed out by the liquid. When radioactive heating naturally reduced the sodium present in this liquid would then have formed part of the icy matrix. Therefore if neutral sodium is found within the icy matrix of the comet nuclei, or neutral sodium within the tail may be determined to have its origins in icy cometary material, it could indicate that aqueous alteration occurred in cometary material in the protosolar nebula. If the neutral sodium emission is partly found to originate in icy cometary material then the relative abundances of neutral sodium from dust and neutral sodium from ice, could also indicate the amount of radiogenic heating that occurred to a particular comet whilst in the protosolar nebula.

### 1.2.1 Sodium in the Solar System

In addition to the sodium observed at comets, it has also been observed in many other bodies in the Solar System. Earth’s atmosphere contains sodium, which is believed to originate from meteorite impacts [Combi et al., 1997]. This complicates the interpretation of ground based sodium emission measurements.

A neutral sodium tail and sodium ion pick-up were also detected at Mercury [Baumgardner et al., 2008; Sarantos et al., 2009]. Furthermore observations of Earth’s Moon showed a bright sodium D line feature in the anti-sunward direction, characteristic of a neutral sodium tail [Matta et al., 2009].

Sodium was also discovered in the atmosphere of Jupiter’s moon, Io [Thomas, 1992]. Despite the relatively small abundance it has been studied extensively at Io, as it is easily detected and is also an important tracer of atmospheric interactions with the plasma torus [Thomas, 1992]. Io is heavily volcanic and provides a constant flow of
particles into Jupiter’s magnetosphere that are subsequently ionised. This was known to produce two distinct regions of plasma: a banana shaped cloud orbiting with Io and a jet close to Io, but the precise dimensions of these two objects were unknown until sodium was detected in the system using the AEOS telescope in Maui [Mendillo et al., 2007]. Only trace amounts of sodium were detected in this system, but as the sodium doublet emission is highly efficient and detectable from Earth, it allowed characterisation of these two different regions providing insight into the overall neutral-plasma budget.

The detection of sodium has also proved important in the Saturn system. The abundance of sodium is expected to be high in long-lived oceans in contact with a rocky core, so when Cassini detected sodium in the plumes of material ejected from Enceladus it was suggested that the material must originate from vast liquid oceans just under the icy surface [Postberg et al., 2009]. To date no significant sodium emission has been detected in this system from Earth, which has led some authors to suggest the mechanism for release of the plume material may not be as simple as release from a near-surface geyser through cracks in Enceladus’ crust [Schneider et al., 2009].

1.2.2 Sodium in Comets

Cometary spectra were first recorded photographically in 1881 and the first cometary detection of sodium D lines occurred in the spectrum of comet C/1881 K1 [Brandt and Chapman, 2004]. The Doppler shift of these lines was originally used to calculate the first estimate of the radial velocity of a comet and by 1900, cometary comae were shown to contain the following features [Brandt and Chapman, 2004]:

1. Swan emission bands of $C_2$
2. Violet emission bands of $CN$
3. $C_3$ emission at 4050 Å
4. $CH$ emission at 4310 Å
5. Sodium D doublet, usually only detected when comets approach near to the Sun
6. Continuous solar spectrum (strongest Fraunhofer lines still apparent)

In some cases the atom responsible for the emission was initially unclear until appropriate laboratory measurements could be obtained, particularly as there was no established theory on the production of atomic and molecular spectra at this time. Even when atomic and molecular theory (see chapter 2.2) were well understood, issues arose in deducing the cometary species present as laboratory spectra often did not match cometary spectra and the intensity distribution varied dramatically between comets (and even between measurements of the same comet taken at different heliocentric distances).
The first comprehensive study of the morphology of neutral cometary sodium tails was made possible by the comprehensive study of Comet C/1995 O1 (Hale-Bopp) during its perihelion passage in 1997. Following the initial detection image, many observations (both spectra and imaging) were performed. Most of the current understanding of neutral sodium tails at comets is a direct result of the extensive campaign of observations taken at comet Hale-Bopp. As the understanding of the observations of the neutral sodium tail at comet Hale-Bopp is so crucial to this field, they are discussed in detail in chapter 2. Observations of other comets at which neutral sodium tails have been observed are also discussed in chapter 2.

Sodium tails have been speculated to have been present at many comets since Hale-Bopp. A list of the comets of interest to this study is given in table 1.2. The instruments that observed the comets of interest to this study are discussed in more detail in chapter 3. The work presented in this thesis mainly focusses on imaging (CoCam imaging [Cremonese et al., 1997b] for comet Hale-Bopp and LASCO imaging [Brueckner et al., 1995] for the other comets listed in the table), but we also consider spectra taken at comet Hale-Bopp.

<table>
<thead>
<tr>
<th>Comet</th>
<th>Designation</th>
<th>Perihelion Date</th>
<th>Sodium Tail</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hyakutake</td>
<td>C/1996 B2</td>
<td>1 May 1996</td>
<td>Predicted, unclear</td>
</tr>
<tr>
<td>Hale-Bopp</td>
<td>C/1995 O1</td>
<td>1 April 1997</td>
<td>Observed</td>
</tr>
<tr>
<td>NEAT</td>
<td>C/2002 V1</td>
<td>18 February 2003</td>
<td>Apparently Observed</td>
</tr>
<tr>
<td>McNaught</td>
<td>C/2006 P1</td>
<td>12 January 2007</td>
<td>Apparently Observed</td>
</tr>
</tbody>
</table>

Table 1.2: Table showing all comet current of interest to the study of cometary sodium tails presented in this thesis. Perihelion dates obtained from NASA/JPL Horizons database [Giorgini et al., 1996]

### 1.3 Aims and Approaches of this Thesis

The principal aims of this thesis are to provide the reader with an overview of the current understanding around neutral sodium observations in comets, discuss how this theoretical understanding has been used to develop the first fully heliocentric distance and velocity dependent model to simulate neutral sodium in comets, known as COMPASS (see chapter 5), and to apply COMPASS to observations of cometary sodium.

The hope is that in developing COMPASS, we have developed a suitable tool for understanding cometary sodium observations that will ultimately provide conclusive evidence of the source of neutral sodium in different comets, and consequently the chemical and physical processes occurring in comets that are responsible for producing sodium D line emissions and additional insight into the composition and structure of the cometary nucleus.

The author initially studies the neutral sodium tail of comet Hale-Bopp (C/1995 O1)
Aims and Approaches of this Thesis

by comparing the results of COMPASS with the results of spectra and imaging studies, as comet Hale-Bopp’s neutral sodium tail remains the most studied to date. Using the results of this initial ‘proof of concept’ study we apply COMPASS to the neutral sodium tails observed close to the Sun by SOHO using the LASCO coronagraph. We find that overall the $1/r^2$ neutral outflow source implemented in COMPASS provides a good match with the available data. As this distribution is consistent with a source of neutral cometary sodium predominantly in cometary dust, we therefore wish to test whether a true dust tail source in COMPASS produces more accurate results. We therefore use a Finson and Probstein [1968] model as a dust tail source analogue for our COMPASS simulations of the observation of comet Hale-Bopp taken using the CoCam instrument in order to determine whether a dust tail source is also consistent with this observation.

This thesis is arranged such that, following the introduction to cometary physics and cometary neutrals presented in chapter 1, it first discusses the theoretical background and observational evidence considered in the development of COMPASS in chapter 2. We then discuss in detail the instrumentation that produced the observations we chose for comparison with COMPASS in this thesis in chapter 3. We then discuss the previous modelling approaches that have increased our understanding of neutral sodium tail observations at comets in chapter 4, in order to provide context and explain why a new model was required. The Brown et al. [1998] model is discussed in detail as it was used as the basis for development of COMPASS. An outline of COMPASS is then discussed in chapter 5, followed by the applications of COMPASS to comet Hale-Bopp (chapters 6, 7 and 8) observations and LASCO observations of near-Sun comets (chapter 9). Finally we put our results into context and draw conclusions on the likely source of sodium in comets based on the work presented in this thesis in chapter 10.
Chapter 2

Review of the Formation of Neutral Sodium Tails at Comets

2.1 Introduction

In this chapter we present a thorough review of the understanding of the formation of neutral sodium tails at comets as it stood prior to the work presented in this thesis. The basic background of the theory required to understand this work is presented in chapter 2.2. We then present a review of the extensive observations of comet C/1995 O1 (Hale-Bopp) in chapter 2.5 and a review of published observations of neutral sodium tails and neutral-sodium-tail-like features observed at other comets in chapter 2.6. The need for a conclusive model that can interpret the observations of neutral sodium tails is highlighted by many of the studies discussed.

2.2 The Theory of the Formation of a Neutral Cometary Sodium Tail

The formation of a neutral cometary sodium tail differs from the formation of ion, dust and other (speculated) neutral cometary tails, due to the presence of neutral sodium in the atmosphere of the Sun and the high efficiency of the sodium D line transition. Resonance fluorescence of solar photons by cometary sodium is the primary process that forms neutral cometary sodium tails.

The neutral atoms are quickly ionised in the sodium tail, primarily by photoionisation due to ultra-violet solar radiation with an approximate (theoretical) lifetime of $1.7 \times 10^5 \text{s}$ [Cremonese et al., 1997b; Zanstra, 1928]. Once the atoms are ionised, resonance fluorescence no longer remains the dominant process and other processes become important, such as mass loading of the solar wind with cometary ions. We have yet
to observe the transition of newly ionised sodium to the ion tail, which suggests rapid ion pick-up. However a lack of observations of this phenomenon may also result from the issue that any such transition would be very difficult to detect due to the difficulty in performing observations (the ion and dust tails can often lie very close together and the background ionised sodium emission is negligible in comparison to that of the more abundant water ions).

The same resonance fluorescence that occurs with sodium may occur with other neutral atoms in the cometary environment, forming neutral tails containing other species. The absorption lines present are dependent upon the energy levels in the atom concerned and therefore other neutral tails are potentially more difficult to observe, as the process is unlikely to be as efficient as that of the sodium D lines. Despite this difficulty some observations suggest the possibility of other neutral cometary tails - particularly for iron [Fulle et al., 2007], although the mechanism for this is suggested to be non-resonance fluorescence rather than resonance fluorescence as for sodium [Zanstra, 1928].

**The Fraunhofer Spectrum** The solar atmosphere contains many neutral elements, which absorb solar photons at characteristic absorption wavelengths corresponding to atomic transitions, prior to the radiation exiting the Sun’s surface. This process causes discrete gaps in the solar spectrum, as the output radiation at these wavelengths is significantly reduced. Figure 2.1a shows the clearest absorption wavelengths in the solar spectrum, known as the Fraunhofer lines [Larson, 2013]. Neutral sodium absorption is responsible for one of the strongest Fraunhofer lines, the D doublet (D1 at 589.6 nm and D2 at 589.0 nm) [Nave, 2012]. The D1/D2 lines are caused by photons being absorbed by electrons in the 3s$^1_{1/2}$ state, causing electronic transitions between the 3p$^1_{1/2}$/3p$^3_{3/2}$ states respectively [Nave, 2012]. This process is demonstrated schematically in figure 2.1b. The 3p level is split into two states due to the interaction between orbital angular momentum and electron spin termed ‘spin-orbit coupling’.

The absorption process involves resonance fluorescence in sodium as when an incident photon is absorbed it promotes an electron and the electron drops directly back to the ground state, emitting a photon with an identical wavelength to the photon absorbed. This is not pertinent to our discussion of sodium tail formation, as the photons resulting from the fluorescence process are emitted isotropically and so do not cause a net acceleration, but is mentioned here for completeness. However, a net acceleration does result from the initial absorption.

**Heliocentric Velocity Dependent Acceleration** The neutral atoms produced at the comet have the same resonant absorption wavelengths as their solar counterparts and therefore the same ‘predisposition’ to preferentially absorb photons at those wavelengths. If a photon is incident on a sodium atom it will exert a force that will result in an acceleration away from the photon’s source. The case is more complicated if solar
(a) Fraunhofer lines in solar spectrum [Larson, 2013]. The sodium doublet is labelled D.

(b) Atomic transition resulting in sodium doublet [Nave, 2012].

**Figure 2.1:** Characteristics of sodium absorption in the solar spectrum.

radiation is incident on the sodium atom due to the Fraunhofer D1 and D2 lines.

If the sodium atom in question has no velocity with respect to the source of the solar radiation (i.e. no heliocentric velocity) then very few solar photons will have a wavelength in the resonant band required for absorption (due to the Fraunhofer sodium D lines) and therefore there will be no significant anti-solar acceleration. However, if the sodium atom has a large positive or negative heliocentric velocity then the solar spectrum will be Doppler shifted with respect to the sodium atom and therefore there will be a larger number of photons at its resonant absorption wavelengths. This will result in an enhanced radiation pressure and consequently a more significant anti-solar acceleration. Therefore the heliocentric velocity of a sodium atom directly determines its acceleration. A schematic of this process is given in figure 2.2.

As the profile of both the D1 and D2 Fraunhofer lines is relatively broad, the magnitude of the heliocentric velocity directly corresponds to the magnitude of the anti-solar acceleration imposed on the sodium atom. This effect, where the velocity of a body determines its acceleration, is a challenge to both the interpretation of observations and successful modelling. In reality sodium atoms will be produced with a distribution of heliocentric velocities and so understanding the variation in acceleration this produces is key to understanding the sodium tail morphologies observed.
The Swings and Greenstein Effects and $G$ Factor Traditionally, the variation in velocity is separated into two distinct effects: the Swings effect, which produces a variation in acceleration due to the relative velocity of the comet with respect to the Sun, and the Greenstein effect, which produces a variation in acceleration due to the relative motion of the individual sodium atoms with respect to the nucleus as the cometary coma expands [Swings, 1941]. This approach can be valuable in treating the broad and narrow features present in the spectra observed separately, but is not required for simulation as both effects can be simulated identically.

The $g$ factor can be calculated using the oscillator strength of the transition and the solar spectrum [Furusho et al., 2005]. The absorption oscillator strength, $f$, of a transition represents the relative intensity (or probability) of an atomic absorption occurring. The absorption oscillator strengths of the sodium D1 and D2 lines are given in table 2.1.

<table>
<thead>
<tr>
<th>Transition</th>
<th>Vacuum Wavelength (nm)</th>
<th>Absorption Oscillator Strength</th>
</tr>
</thead>
<tbody>
<tr>
<td>D1</td>
<td>589.756 661 7(15)</td>
<td>0.3199(13)</td>
</tr>
<tr>
<td>D2</td>
<td>589.158 326 4(15)</td>
<td>0.6405(11)</td>
</tr>
</tbody>
</table>

Table 2.1: Table showing vacuum wavelengths and absorption oscillator strengths for the two sodium D line transitions [Steck, 2000].

A solar photon may be absorbed in the sodium D transition if its incident, Doppler-shifted wavelength is equal to that of the D1 or D2 transition. The observed wavelength, $\lambda_{\text{obs}}$, resulting from a relativistic doppler shift of rest wavelength, $\lambda_{\text{rest}}$, by radial velocity, $v_r$, of a source moving away from the observer is given by Bradley W. Carroll [1996]:

$$\lambda_{\text{obs}} = \lambda_{\text{rest}} \left( \frac{1 - \frac{v_r}{c}}{1 + \frac{v_r}{c}} \right)$$
\[ \lambda_{\text{obs}} = \lambda_{\text{rest}} \sqrt{\frac{1 + (v_r/c)}{1 - (v_r/c)}} , \] (2.1)

where \( c \) is the speed of light. In the case of solar radiation incident on a sodium atom the radial velocity under consideration is the heliocentric velocity (i.e. we may consider a stationary source and a moving sodium atom). Therefore it is possible to calculate the heliocentric sodium atom velocity required for each wavelength of the solar spectrum to be absorbed in the sodium atom D1 and D2 transitions. In this way we may calculate the intensity of solar radiation (i.e. number of photons) as a function of heliocentric velocity that may be absorbed by the sodium D1 and D2 transitions. Combining this function with the oscillator frequency, which represents the probability of an incident photon at that wavelength results in an absorption, results in the \( g \) factor for the sodium D1 and D2 transitions as a function of heliocentric velocity. Then summing the two \( g \) factors for D1 and D2 results in an overall \( g \) factor for the efficiency of the sodium D line transition. Therefore the overall \( g \) factor, which characterises the resonant fluorescence of the sodium D line absorption due to solar radiation, is a function of the heliocentric velocity of the sodium atom.

The effect of resonance fluorescence on neutral sodium atoms was first discussed in detail during studies of the neutral sodium cloud surrounding Io. Smyth [1979] state that a sodium atom absorbing a photon of energy \( h\nu \) in either the D1 or D2 lines would gain a momentum of \( h\nu_i/c \) (where \( i = 1, 2 \) for D1, D2 respectively) in the anti-sunward direction. The excited neutral sodium atom would then return to its ground state approximately \( 10^{-8} \) seconds later via the emission of a photon, and it would experience a second momentum change of the same magnitude but randomly directed. Smyth [1979] state that the rate, \( J_i \), (equivalent to the \( g \) factor) by which a neutral sodium atom absorbs photons in the D1 and D2 lines is given by:

\[ J_i = \gamma(v) \frac{\pi e^2}{m_e c} \frac{\pi F_{\nu_i}}{h\nu_i} f_i R^{-2} , \] (2.2)

where \( R \) is the heliocentric distance in AU, \( f_i \) is the oscillator strength of the \( i \)th line, \( (\pi F_{\nu_i}) \) is the solar continuum photon energy flux between the D1 and D2 lines at 1 AU and \( \gamma(v) \) is the fraction of this solar flux now available to the sodium atom due the heliocentric velocity of the sodium atom Doppler shifting the incident solar radiation out of the deepest spectral regions of Fraunhofer absorption. The acceleration, \( b \), experienced by the sodium atom is therefore [Smyth, 1979]:

\[ b = \frac{1}{m} \left( \frac{h\nu_1}{c} J_1 + \frac{h\nu_2}{c} J_2 \right) \] , (2.3)

where \( m \) is the mass of the sodium atom.
The Stagnation Region  An interesting effect is observed if the sodium atom is produced on the sunward side of the nucleus with a positive velocity in the sunward direction, counteracting the heliocentric velocity of the nucleus. In this instance the acceleration due to solar radiation pressure will be in the opposite direction to the velocity. However, a decrease in heliocentric velocity results in a decrease in the anti-sunward acceleration. Therefore the sodium atom’s velocity will approach zero and so too will its acceleration, resulting in the sodium atom appearing to pause on the sunward side of the nucleus. This situation is highly unstable to perturbations, but if enough sodium atoms are initially produced in this way it can result in a build up of sodium atoms on the sunward side of the cometary nucleus, known as the stagnation region. This region would be very difficult to observe because the sodium atoms contained within it would have low velocities and consequently not significantly absorb (and re-emit) solar photons.

The stagnation region is a direct consequence of the dependence of radiation pressure on the heliocentric velocity of the sodium atom. It was first observed by Brown et al. [1998] at comet Hale-Bopp, and this observation is studied in more detail in chapter 6 (and is reproduced in figure 6.1).

2.3 General Methods of Releasing Neutral Sodium from Cometary Material

The source of neutral cometary sodium currently remains unknown, or at least uncertain. The evidence for different theories is presented in the remainder of the sections in this chapter, but there are certain aspects of the physics of these processes that must be discussed. In this chapter we do not consider the likelihood of each of these formation processes, but present each as the initial options to be supported or rejected by observational evidence. The list discussed here is expanded from that presented by Schmidt et al. [2015].

Sputtering  Sputtering is the process of releasing material from the surface of a body caused by the continuous bombardment of fast atoms or ions. Sputtering is usually considered to be a multi step process, where one initial collision results in a ‘cascade of collisions’ that then release material from the surface of a body [de Pater and Lissauer, 2001]. Ions are more likely to have higher velocities than atoms as they may be accelerated by electric fields, whereas atoms may only be accelerated by collisions. Therefore sputtering is more likely to be caused by ions that atoms. During sputtering, the energy and momentum of the incident ions are transferred to the surface layers of the material, such that particles sputtered by ions tend to have an energy distribution that extends from thermal energies to high energies, typically as $E^{-2}$ [Townsend,
Sputtering by solar wind ions is potentially an important mechanism for release of cometary sodium from the nucleus of a comet.

**Photo-sputtering** Photon induced sputtering, or photo-sputtering, is also known as photon stimulated desorption, or photo-desorption, and is sputtering induced by photons incident on the material. When photons impact the surface of a material, their energy is absorbed by an atom on the surface (which itself is part of a neutral solid). This atom is then excited to a new state where its attraction to the material is reduced. In its new excited state, the thermal energy of the atom may then be sufficient for it to escape from the solid. Photo-sputtering is therefore the result of electronic excitations, rather than thermal processes (thermal desorption) or momentum transfer (ion or atom sputtering). As electrons do not have large masses, their momentum is also usually relatively small, and the electronic excitations induced by photons may also be induced by electrons so photo-sputtering produces similar distributions as sputtering by electrons.

Atoms emitted via photo-sputtering are generally of lower energy than those emitted by sputtering of atoms or ions, as they tend to have approximately the thermal energy of the material from which they were sputtered. It has been shown experimentally by Yakshinskiy and Madey [1999] that only ultraviolet photons with energies greater than 4eV cause detectable desorption of sodium from surfaces that simulate lunar silicates, which may be similar to cometary material. Photo-sputtering by solar ultraviolet photons is potentially an important mechanism for the release of cometary sodium from the surface of the nucleus. Leblanc et al. [2008] suggest that their observations of comet McNaught are consistent with neutral sodium released via sputtering or photo-sputtering.

**Thermal Desorption** Photons hitting the cometary nucleus in sufficient quantities will cause energy to be imparted to the ice which will sublimate it. This sublimating material is a key feature of the cometary environment (as discussed in chapter 1) and could also be the mechanism by which neutral sodium atoms are emitted from cometary material by the process of thermal desorption. Thermal desorption is the process by which atoms or molecules are randomly emitted from the surface of a material due to the random thermal energy of atoms in it being such that the thermal energy of one atom is sufficient for it to overcome the potential of the material and escape. Furusho et al. [2005] speculate that thermal desorption from dust grains could be the mechanism by which neutral sodium was released based on observations of comet Hale-Bopp.

**Dissociative Recombination** Dissociative recombination occurs when a molecular ion splits apart upon recombination with an electron, producing two neutral fragments. Dissociative recombination of sodium bearing molecular ions, for example NaOH is
potentially an important mechanism for release of cometary sodium. This method of neutral sodium production was supported by Combi et al. [1997] based on their observations of comet Hale-Bopp.

**Molecular Dissociation with long dissociation lifetimes** The dissociation, or splitting, of molecules containing neutral sodium may be an important mechanism for neutral sodium release within the central cometary coma [Whipple and Huebner, 1976]. Sekanina [1997] speculate that sodium containing molecular parents could have been released from the dust entrained in the outflowing sublimated gas, and that they should have relatively long dissociation lifetimes to survive sufficiently in the neutral sodium tail. They suggest this as a possible source of neutral sodium tail production at comet Hale-Bopp.

**Collisions between dust and very small grains** In a similar mechanism to sputtering, impacts between individual cometary dust particles of different sizes, which have been released from the cometary nucleus via sublimation of the surrounding ices, may result in release of the neutral sodium atoms contained within the dust particles. This mechanism could produce an ‘impact vapour’ that contained neutral sodium and was first speculated by Ip and Jorda [1998] based on their observations of comet Hale-Bopp.

### 2.4 Neutral Sodium Observations before Comet Hale-Bopp

Following the initial detection of sodium D lines in the spectrum of comet C/1881 K1, sodium D line emission detection was reported in the Great Comet of 1882 by Levin [1964] and Zanstra [1928], who used these observations to deduce that the emission was due to resonance fluorescence (i.e. that the solar radiation was being absorbed by cometary material and then re-emitted to produce the features observed in the coma). Zanstra [1928] also suggested that non-resonant fluorescence was responsible for the iron spectral line observed in the Great Comet of 1882 (i.e. in this case the emitted wavelength was longer than the incident wavelength).

Newall [1910] observed that sodium D line emission in comet 1910a exceeded that of the $C_2$ Swan band, using a direct-vision prism between the eye and the eyepiece of a 25 inch telescope. This observation had the potential to identify a distinct sodium tail but no such feature was reported [Combi et al., 1997]. In 1911 Schwarzschild and Kron used a similar mechanism to Zanstra to explain these observations of the cometary tail, suggesting that the sodium light observed was the result of resonance fluorescence [Schwarzschild and Kron, 1911].
Nguyen-Huu-Doan [1960], recorded a seven degree neutral sodium tail at comet Mrkos (C/1957 P1), using a Schmidt camera with an objective prism. The sodium tail was identified through multiple spectroscopic measurements of sodium D line emission at different positions, however no detailed description of the morphology nor speculation into the processes that caused these features was presented.

In the years that followed this discovery sodium D line emission was also observed in other bright comets such as Ikeya-Seki (C/1965 S1), Bennet (C/1969 Y1), Kohoutek (C/1973 E1), West (C/1976 V1) and Halley (1P) but due to viewing conditions (the field of view usually subtended only a few $10^5$ km) it was impossible to detect sodium in the comet’s tail [Combi et al., 1997; Cremonese, 1999; Spinrad and Miner, 1968; Oppenheimer, 1980; Rahe et al., 1976]. Low activity comets do not typically have observable neutral sodium tails, indeed the furthest heliocentric distance at which neutral sodium emission has been detected is approximately 1.4 AU, by Oppenheimer [1980] in comet West (C/1976 V1). Oppenheimer [1980] suggested from their observations of comet West at 1.4 AU that an icy matrix source of cometary sodium was the most likely because the cometary dust would be too cold at this heliocentric distance to release neutral sodium via sublimation.

2.5 The Neutral Sodium Tail of Comet Hale-Bopp

The observations of comet Hale-Bopp constitute the main source of data that has contributed to our understanding of neutral sodium in comets. In this chapter we review the literature relevant to these observations. We focus primarily on the studies of Cremonese et al. [1997b], Brown et al. [1998] and Rauer et al. [1998] as they form the central data sources for the study of neutral sodium at comet Hale-Bopp presented in this thesis. Relevant studies are discussed in roughly the order they were performed, and the dates of each observation taken is given in table 2.2, section 10.1.

Neutral sodium emission in comet Hale-Bopp was first detected by Kawabata and Ayani [1997] at the Bisei Astronomical Observatory. Their results were not published, but their preliminary analysis seemed to indicate that the sodium emission was more extended towards the dust tail of the comet.

The initial detection of a clearly distinct neutral sodium tail at comet Hale-Bopp in CoCam images by the Cremonese et al. [1997a] (taken during 16-22 April) ignited interest in the field. The Hale-Bopp team’s IAU circular prompted other authors to attempt to observe neutral sodium in the comet and investigate whether it had been detected in previous observations. Discovering the mechanism by which neutral sodium was produced was the main goal of these subsequent works, as this could potentially allow insight into how comets were formed in addition to giving more details about the properties of an active comet environment.
Cremonese et al. [1997b] performed high resolution spectroscopy at several points along the tail using the 4.2m William Herschel Telescope on 19.9 UT, 20.9 UT and 23.9 UT April 1997 with the Utrecht Echelle Spectrograph in both standard echelon mode and with the narrow band sodium filter used in CoCam inserted in the spectrograph. Surface brightnesses were determined from spectroscopic data but could not be obtained from CoCam images due to difficulty in accurately calibrating these wide field images.

Cremonese et al. [1997b] explained the structure and brightness of the observed sodium tail using simple theoretical calculations based on the Finson and Probstein [1968] model of the dust β (defined in equation (1.1)), average emitted intensity due to sodium production and the efficiency of the sodium emission (and recently updated photoionisation lifetimes at 1 AU from Huebner et al. [1993]). Using these assumptions, Cremonese et al. [1997b] estimate the best fitting syndyne of the neutral sodium tail in the CoCam images to be \( \beta = 82 \pm 3 \). This value was so high that it implied that only atoms could be responsible for this emission (not molecules or dust - as the largest reported value for these species is \( \beta = 2 \)). From consideration of the radiation pressure due to resonance fluorescence and gravitational forces acting on the atom, Cremonese et al. [1997b] calculate that any molecules at the location of the neutral sodium tail syndyne must have a mass of \( 22 \pm 1 \) amu and therefore that the tail must be composed of neutral sodium atoms, not molecules containing sodium (sodium atom mass = 22.98977 amu [Bentor, 2016]).

Cremonese et al. [1997b] were unable to determine the source of sodium at comet Hale-Bopp but suggested that the distinct neutral sodium tail they had observed was the result of fluorescence of sodium atoms that had been released at or near the nucleus, rather than at the neutral sodium tail’s current observed position because of the relatively high velocities observed. Cremonese et al. [1997b] also noted that they expect the sodium tail to vary strongly with observing geometry and cometary heliocentric velocity, possibly producing different sodium distributions at different observation dates. Cremonese et al. [1997b] use their results to estimate the production rate, \( Q(Na) \), of neutral sodium at Hale-Bopp to be \( Q(Na) \approx 5 \times 10^{25} \) atoms s\(^{-1} \), based on the same consideration of column density and \( g \) factor as presented in Chamberlain and Hunten [1987]. Their modelling also supported a much longer value of the characteristic lifetime against photoionisation for neutral sodium (approximately 2 days at 1 AU) than had previously been collated by Huebner et al. [1992]. Cremonese et al. [1997b] used a value approximately three times higher than that typically used at planetary atmospheres at the time (e.g. the Moon and Io), and is now the generally accepted value for photoionisation lifetime of neutral sodium at 1 AU in the cometary environment.

Wilson et al. [1998] performed large field of view multi-wavelength observations of the sodium tail of comet Hale-Bopp using the McDonald Observatory in Texas in 17 and 20 March 1997. The images were taken using a range of different filters to allow detection of different species, each with a spectral width of approximately 7 Å. Filters centred on
5893 Å, 6199 Å and 6050 Å were chosen to allow detection of the sodium D lines, a $H_2O^+$ emission line and the off-band continuum respectively. Following bias subtraction, flat fielding, normalisation to single exposure time, subtraction of background scattered light from the sky and correction for atmospheric extinction, the images were further processed by removal of the 6050 Å images from the Na and $H_2O^+$ filter images to remove the dust continuum from the sodium filter images and the ion tail filter images.

The sodium tail observed by Wilson et al. [1998] had a different direction from the ion tail, dust tail and sodium tail seen by Cremonese et al. [1997b] (recorded approximately one month later). Wilson et al. [1998] interpreted these results as an indication that the sodium tail at Hale-Bopp was highly variable. To account for the morphology of the sodium tail they observed, Wilson et al. [1998] suggest that there must be an extended source of sodium atoms tailward of the cometary nucleus. However, they disagree with the results of Combi et al. [1997], suggesting that the observed sodium tail could not be formed by release of sodium by recombination or dissociation processes in the ion tail, as their brightest sodium emission coincides with the dust tail, not the ion tail (see figure 2.3). Instead they propose the release of sodium atoms from grains in the dust tail as a mechanism for its formation.

They also found the sodium tail of comet Hale-Bopp to be more extended in width than either the dust or ion tails, in contrast to the results of Cremonese et al. [1997b], which showed that the sodium tail contained a bright, narrow component. As this bright, narrow component was not present in their data, Wilson et al. [1998] suggest that the nuclear source required to produce it must have commenced or become dominant between March 1997 and April 1997. It may also be significant that comet Hale-Bopp’s perihelion occurred on 1 April 1997.

The study by Combi et al. [1997] focuses on observations of cometary sodium before Hale-Bopp at comets and the implications their work has on the preliminary observations of neutral sodium at Hale-Bopp previously presented.

Combi et al. [1997] study the spacial profiles of neutral sodium at different displacements from the comet nucleus along the Sun-comet line (and at the comet nucleus across the tail and at an angle to it) observed at comets C/1969 Y1 (Bennett), C/1973 D1 (Kohoutek) and 1P (Halley). They find:

- A bifurcated structure (as seen in the ion tail but not in the dust tail).
- A flattened slope in the antisunward profiles (decrease of $1/r$ close to the comet nucleus, but then decreases at a much lower rate).
- Wave-like structures in many of the antisunward profiles.
- Side lobes in the nucleus-centered cross-tail profiles.

and suggest that these observations (reproduced in figure 2.4) are consistent with a major fraction of gaseous sodium seen in long-slit spectroscopic observations being
Figure 2.3: Plot showing a comparison between the positions of the ion, neutral sodium, and dust tails at comet Hale-Bopp, which Wilson et al. [1998] took to indicate that the position of the neutral sodium tail was incompatible with its production in the ion tail. Neutral sodium is indicated by the yellow contour in the central panel. Image reproduced from Wilson et al. [1998], see this paper for more details.

produced by an extended plasma source in the tail. The bifurcated structure is also seen in the ion tail spectra in figure 2.4, but is not present in the dust continuum spectra.
Combi et al. [1997] also created a model (discussed in more detail in chapter 4) to investigate the source of neutral sodium. They found that the relatively flat profiles (less steep than $1/r$) observed in the neutral sodium tail are inconsistent with their model if a nucleus source is used, as this never produces a spatial profile with less than a $1/r$ decrease. Combi et al. [1997] therefore suggest that these observations can only be explained using at least two sodium sources: a combination of a point source releasing sodium atoms directly from the nucleus (or a short lived ($10^3$ s) parent molecule very near the nucleus) and an extended plasma source. Combi et al. [1997] also note that
the plasma environment of comet Hale-Bopp is possibly very different to the comets in their study, as the ionosphere of Hale-Bopp is much larger. They consider the plasma source of neutral sodium to be highly variable but up to four to five times stronger than the nucleus source based on their observations of the tails and their flanks. Combi et al. [1997] also note the observations of neutral sodium released from vaporised dust in near-Sun comets considered by Huebner [1970], and suggest that although a dust source is inconsistent with their results it is likely to form a key part of neutral sodium release at comets with relatively small perihelia.

Combi et al. [1997] suggest dissociative recombination of a molecular ion as a likely parent to the sodium atom emissions observed, and suggest the primary parent is likely to be a nucleus ice (not dust) source. Combi et al. [1997] consider dissociative recombination of a molecular ion:

\[ \text{NaX}^+ + e^- \rightarrow \text{Na} + X, \]  

(2.4)

to be more likely than radiative recombination of an ionised neutral sodium atom:

\[ \text{Na}^+ + e^- \rightarrow \text{Na} + \text{photon}, \]  

(2.5)

because the cross section for dissociative recombination of a molecular ion is much higher than radiative recombination of \( \text{Na}^+ \) and radiative recombination is considered to be very inefficient in the cometary environment [Johnson, 1994]. Furthermore, they suggest that the molecular parent of this tail is likely to be a plasma source in the ion tail, but as the lifetimes required were longer than that of \( \text{NaOH} \) and suitable laboratory measurements were unavailable they are unable to suggest a potential parent species.

Combi et al. [1997] also state that although dust grains are potentially a source of sodium they could not be responsible for the sodium tails observed at these comets because charged dust grains do not travel along the plasma tail, where they speculate that the neutral sodium observed down the tail originated.

Rauer et al. [1998] observed Hale-Bopp on 14 March 1997 at the Observatoire de Haute-Provence, using the CARELEC spectrograph at the 1.93m telescope and again on 16 April 1997 using the ISIS double beam spectrograph at the 4.2m William-Herschel Telescope of the Isaac Newton Group on La Palma, Spain. The spectra were bias subtracted, flat fielded and wavelength calibrated where possible (non-photometric conditions in April did not allow this). The reflected dust continuum was also subtracted from the spectra. The geometry of the observation was particularly unfavourable so the comet could only be observed close to twilight. Therefore determining the sky contributions was difficult. Sodium atom emissions were also contaminated by telluric water emissions. Rauer et al. [1998] were able to calculate a neutral sodium production rate of
between $3 \times 10^{24} \text{s}^{-1}$ and $5 \times 10^{25} \text{s}^{-1}$ for their observations on 14th March 1997.

Rauer et al. [1998] consider their results to suggest that the extended sodium distribution in the inner coma of comet Hale-Bopp is not in agreement with a pure nuclear source, as in this case a sunward extent of only a few $10^3 \text{km}$ would be expected and they see neutral sodium out to approximately $10^5 \text{km}$ from the cometary nucleus. They also suggest that the observation of an extended sodium cloud can only result from the existence of an extended source or reduction of the tailward sodium acceleration. Rauer et al. [1998] find no relationship between the position of the ion tail and the sodium tail, and so, unlike Combi et al. [1997], they rule out a plasma source for neutral sodium at Hale-Bopp. Instead they suggest a molecular parent (sublimated directly from the nucleus or from dust particles) or the release of sodium directly from dust grains (by sputtering) as potential source. They also suggest that the general sunward/antisunward asymmetry in the coma found for sodium and dust supports the release of sodium from dust particles.

Rauer et al. [1998] also note that care must be taken when comparing the distribution of sodium emission intensities with that of the suspected parent molecules, as strict correlation is not expected due to the large radiation pressure acting efficiently on sodium atoms but not on their prospective parents. They also speculate that if sodium is a second generation species (or the production of sodium is more complex than initially considered) the correlation between the sodium tail and its source would be further diluted. In addition they suggest that the spectral irradiance within the sodium profiles can reach intensity levels comparable to that of the Sun inside the coma and therefore that internal radiative pressure may also be important.

In addition Rauer et al. [1998] state that the secondary maxima seen in their spectra (corresponding to the stagnation region) are less intense in the sodium emission centered on the nucleus of comet Hale-Bopp in their observations than in the comparable dust continuum spectra.

Ip and Jorda [1998] agreed that the large radial velocity of sodium atoms observed by Cremonese et al. [1997b] must be the result of solar radiation pressure. They were ultimately unable to determine the source of sodium at Hale-Bopp without obtaining higher resolution spectroscopic measurements. Ip and Jorda [1998] argue that the relatively small sodium production rate estimated by Cremonese et al. [1997b] is consistent with thermal desorption of neutral sodium atoms (or their parent molecules) from nonvolatile dust grains, even if full sublimation would only occur when the surface temperature exceeds 1500 K (heliocentric distances of 0.05 AU or less).

As Hale-Bopp had a larger dust content than any other comet studied at the time, Ip and Jorda [1998] also suggested that photo-sputtering and ion sputtering may not be the primary sources of sodium production at the nucleus, because of the relatively small estimated production rate of neutral sodium ($5 \times 10^{25} \text{s}^{-1}$) compared to the gas
production rate at comet Hale-Bopp (10^{31} \text{ molecules s}^{-1}) and assuming a cosmic abundance of sodium at \( Na/O = 2.7 \times 10^{-3} \) as given by Allen [1976]. Ip and Jorda [1998] note that photo-sputtering alone is inadequate to explain the observed sodium tail unless cometary material has a significantly higher sodium abundance than lunar surface material, which seems unlikely as the lunar surface contains a significant amount of impacted material from comets and asteroids. Furthermore, estimates for the production rate due to ion sputtering (based on scaled estimates of typical cometary plasma boundary distances) are too small. [Ip and Jorda, 1998] therefore suggest that ion sputtering alone is inadequate to explain the observed sodium tail at Hale-Bopp and conclude that sodium emission must be primarily due to the cometary environment, i.e. dust or cometary ion impact results in the release of sodium atoms or their parent molecules.

Finally Ip and Jorda [1998] suggest that very small grains (10 - 100 \text{ Å}) may be responsible for release of sodium from dust, as their charge to mass ratio results in electromagnetic forces dominating their motion. They would therefore effectively be ‘picked up’ by cometary plasma flow, resulting in dust impacts. Very small grains were extremely abundant in the coma of comet Halley and so Ip and Jorda [1998] suggested the same may be true of Hale-Bopp. The estimated minimum amount of very small grains required to account for the observed production rate at Hale-Bopp indicates that this method of releasing sodium from its parent atoms is feasible based on observations of very small grains in the coma of comet Halley, particularly if grain-grain collisions are also included [Ip and Jorda, 1998].

Arpigny et al. [1998] took spectroscopic measurements of the sodium emission at Hale-Bopp using the Observatoroire de Haute-Provence in conjunction with the ELODIE echelon spectrometer at the 1.93 m telescope. Their experimental setup allowed two spectra to be obtained simultaneously using a pair of optical fibres. Spectra were recorded on the 25-27 March 1997 with the fibres aligned along the Sun-comet line and perpendicular to it and then on 15-17 April 1997 with the fibres aligned along the radial vector.

Again, the dust scattered solar spectrum was subtracted and corrections for the telluric absorptions were applied. No absolute measurements could be obtained from these results as they were not calibrated, but relative intensities could be extracted from the data. Arpigny et al. [1998] suggest that collisional coupling of sodium to water molecules can increase the size of the sodium coma, but estimate that this effect alone is inadequate to explain the full extent of the sodium coma observed at Hale-Bopp. They therefore suggest that the variation in sodium emission intensity they observed in the coma is consistent with a combination of a central source (with collisional entrainment in the densest regions in the coma) with either an extended source or multiple extended sources to account for the size of the sodium coma.

Barker et al. [1997] observed comet Hale-Bopp using the 2D Coudé cross-dispersed
Echelle spectrograph at the f/33 focus of the 2.7m Harlan Smith Telescope at McDonald Observatory on 1 March 1997 and 5 April 1997. Unlike the studies of Cremonese et al. [1997b] in the tail region and Arpigny et al. [1998] in the outer coma, Barker et al. [1997] focused on the inner coma. Due to their high spectral resolution of 1.7 km/s, Barker et al. [1997] were able to investigate neutral sodium emission features in the region directly surrounding the cometary nucleus. Barker et al. [1997] also took observations of hot stars and the solar spectrum to allow removal of telluric water vapour absorption lines and the reflected solar continuum, but because of large uncertainties in the absolute flux calibrations they present their data as relative to the optocentre spectra (corrected for airmass and exposure time). Barker et al. [1997] do not correct for projection effects due to different solar phase angles in the two dates they considered (41.9° on 1 March and 46.2° on 5 April).

Barker et al. [1997] identify two peaks in their spectra, which they attribute to a ‘core’ population of neutral sodium emitted directly from the cometary nucleus and a ‘secondary’ population of neutral sodium emitted from an extended source that must be present at least $2 \times 10^5$ km from the nucleus to be consistent with the results of Brown et al. [1998]. Barker et al. [1997] identify these two features in their spectra and separate them by fitting two Gaussian profiles to the spectra (using the line centres, peak flux levels and FWHM’s as free parameters). From these fits, which are reproduced in figure 2.5, Barker et al. [1997] find that:

1. The centres of the core profiles have Doppler shifts of $\pm 0.7$ km/s, which is consistent with resonance fluorescence.

2. The core population has a narrow velocity distribution of approximately 2 km/s, so must have been produced locally.

3. The core flux profile is significantly greater than the secondary profile flux within $10^4$ km from the cometary optocentre.

4. Velocity dispersions are larger in the secondary profiles than in the core profiles, but in very dusty regions smaller dispersion is present in the secondary profiles.

By considering the core populations taken from the April spectra, Barker et al. [1997] are also able to obtain $D_2/D_1$ line strength ratios that are consistent with the ratio for an optically thin coma (1.67). From this analysis Barker et al. [1997] conclude that the secondary core is likely to have been released from dust, whereas the core population of neutral sodium is likely to have been released directly from the nucleus. Barker et al. [1997] also highlight the need for further modelling in this area because, as the coma of the comet Hale-Bopp is optically thin, integrated velocity distributions throughout the coma are measured in spectra.

Kupperman et al. [1998] observed neutral sodium emission from comet Hale-Bopp on 19 April 1997 between $10^4$ km and $10^6$ km from the comet nucleus using the Ultraviolet and Visible Imagers and Spectrographic Imagers (UVISI) Midcourse Space Experiment,
between the small scales of the Brown et al. [1998] observations and the large scales of Cremonese et al. [1997b] and Wilson et al. [1998] observations. UVISI was slewed (path reproduced in figure 2.6) from the end of the dust tail to the comet nucleus, and using the observations of the spectrographic imagers it was possible to reconstruct spatial images of the sodium, \( \text{H}_3\text{O}^+ \) and dust tails, which are reproduced in figure 2.7. Using this method, UVISI observed a diffuse neutral sodium tail comparable to that seen by Wilson et al. [1998], but not at all like the narrow sodium tail observed three days prior to the Kupperman et al. [1998] observations by Cremonese et al. [1997b].

Kupperman et al. [1998] find that for the mid range scale in their observations, an extended source of neutral sodium is not required and a point source is sufficient to reproduce their observations using the model they have developed. The Kupperman et al. [1998] model is based on that initially presented by Cremonese et al. [1997b], which simulates the emission from a point source of neutral sodium that experiences radiation pressure due to resonance fluorescence, where the intensity along the tail, \( I(r) \) is given by:

\[
I(r) = \frac{10^{-6}Qg(r)}{2v_0t(r)v(r)R^2} e^{-t(r)/R^2\tau},
\]

where \( Q \) is the production rate of sodium atoms (in atoms per second), \( g(r) \) is the \( g \) factor at 1 AU, \( v_0 \) is the initial velocity of the sodium atoms, \( t(r) \) is the time taken by an atom to reach a cometary distance \( r \), \( v(r) \) is the velocity of the neutral sodium atom at cometary distance \( r \), \( R \) is the heliocentric distance in AU and \( \tau \) is the
characteristic lifetime against photoionisation (the dominant process by which neutral sodium atoms cease D line emission as they become ionised). Figure 2.8 shows that this model provides a good match to the observations of Kupperman et al. [1998] down the tail.

The point source assumption required for this model is valid for a source of sodium directly at the nucleus or with a short lifetime, and Kupperman et al. [1998] believe it is best suited to a photodissociation model of neutral cometary sodium released from NaOH.

The Brown et al. [1998] study was the first to combine the suggestions of other authors into a coherent theory for sodium production at Hale-Bopp. It included a relatively sophisticated model to parametrize the Swings and Greenstein effects to allow a thorough interpretation of the available observations. This model was key to understanding the formation of a sodium tail at comet Hale-Bopp and was used as a starting point for this thesis. The details of the implementation of the Brown et al. [1998] model are discussed in chapter 4 but the observations performed by Brown et al. [1998] and their interpretations (resulting primarily from the model outputs) are presented here.

Brown et al. [1998] used observations of the sodium emission of comet Hale-Bopp from the Lick Observatory 0.6m Coudé auxiliary telescope coupled to the Hamilton Echelle
Figure 2.7: Images of the dust (top), sodium (middle) and $H_2O^+$ (bottom) emissions reconstructed data taken by UVISI during the slew across the tail of comet Hale-Bopp performed on 19 April 1997 (see figure 2.6). Reproduced from Kupperman et al. [1998].

Spectrometer on 8 April 1997 and 10 April 1997. Each spectrum was taken using a 6-arcmin slit aligned along the Sun-comet line. They processed the data by subtracting sky and solar continuum reflected dust contributions from the spectra. Brown et al. [1998] were also able to calibrate their data to record quantitative measurements of the cometary sodium velocities and relative sodium intensities by comparison to the bright sodium sky line emission from San Jose, California. Their results showed a sunward increase in intensity, which has since been termed the sunward stagnation region (previously discussed in chapter 2.2). The results of Brown et al. [1998] also show the first indication of a sunward increase in the velocity of neutral sodium atoms in the tail that extends further from the nucleus than the sunward spike. The large sunward velocities they observed can only be the result of an extended source of neutral sodium atoms that exists in that location, because any sodium released at or near the nucleus would have been unable to reach this distance from the nucleus due to the strong effects of resonance fluorescence.

Brown et al. [1998] modelled a plasma source for the sodium atoms based on observed velocities of $H_2O^+$ (extracted from spectroscopic measurements of the ion tail taken on
six nights between 8 March and 5 April 1997 using the method described by Brown et al. [1994]). Their model of the plasma tail was one dimensional and so could not account for the three dimensional motion of sodium atoms travelling through the dense cometary coma, or consequently the tailward sodium atom observations. Their interpretation is therefore confined to the region on the sunward side of the nucleus. Despite this limitation, their results clearly imply that the high initial velocities of the ions within ion tail are incompatible with the theory of sodium production from a plasma source within the ion tail. The best fit to their observations was obtained using a combination of 55% from a nuclear point source and 45% from an extended \(1/r^2\), higher velocity) source in the dust. They also calculate that no more than 5% of the observed sodium can come from the plasma source suggested by Combi et al. [1997].

Kawakita and Fujii [1998] observed Hale-Bopp on 17.82 March 1997, (just after the observation performed by Wilson et al. [1998]) and on 19.45 April 1997 (between the observations of Cremonese et al. [1997b] on 16.88 April 1997 and the observations of Ip and Jorda [1998] on 2.82 May 1997) using the low-dispersion spectrograph mounted on the 0.28m Fuhii-Bisei Telescope. Kawakita and Fujii [1998] extracted the emission of cometary sodium D lines by removing the solar continuum emission and the telluric sodium emission (using both the lunar and sky spectra for each subtraction).

The results of the Kawakita and Fujii [1998] study are consistent with other studies in that before perihelion (1st April 1997) they observed a diffuse sodium tail and no narrow sodium tail, whereas after perihelion both narrow and diffuse sodium tails were observed. Kawakita and Fujii [1998] agree with previous theories for the origin of the diffuse sodium tail in the dust tail, but investigate the narrow sodium tail further.
Kawakita and Fujii [1998] do not accept the theory presented by Wilson et al. [1998] that the production of the nuclear or near nuclear source increased resulting in the observed change in morphology, and produce a Monte Carlo simulation to model the distribution if this was the case. From the results of their simulation Kawakita and Fujii [1998] conclude that the morphological change observed in the narrow sodium tail was primarily a result of the dependence of the radiation pressure and \( g \) factor on the heliocentric velocity of the sodium atoms, not on a change in the production rate of the nuclear (or near nuclear) source. In their letter, Kawakita and Fujii [1998] also note that the change of morphology may be due to a difference in observing geometry (as first speculated by Cremonese et al. [1997b]), which was not accounted for in their results. This again highlights the need for a model capable of including the effects of orbital motion and observational perspective.

Cremonese and Fulle [1997] review the works of other authors to draw a more conclusive picture of the morphology and variability of neutral sodium tail(s) at comet Hale-Bopp. Cremonese and Fulle [1997] present high resolution spectroscopic results along the neutral sodium tail, which are reproduced in figure 2.10, that were taken using the William-Herschel Telescope with the Utrecht Echelle Spectrograph with a slit width of 1.1 arcsec at different cometocentric distances as shown in figure 2.9. The largest peaks in both spectra are that of the telluric sodium doublet, which highlights that the spectra have not been correctly calibrated as the telluric neutral sodium D1 and D2 lines should be at 589.6 nm and 589.0 nm respectively, not at 589.5 nm and 589.0 nm as they appear in the figure. This has been discussed by Cremonese and Fulle [1997] and was apparently the result of a calibration error. The overall shape of the spectra remains correct.

Both spectra in figure 2.10 show fast and slow Doppler shifted peaks (labelled F and S respectively), but are very different - highlighting the dependence of the measurements on the position at which they were taken in the coma. Based on the results of previous analysis, Cremonese and Fulle [1997] interpret the slower peak as due to sodium atoms released locally from dust particles and the faster peak as being due to the sodium atoms coming from the nuclear region (that had already been accelerated by resonance fluorescence and therefore had greater velocities). The plot in figure 2.10b shows the S peaks merging into the F peaks, as the slower peak is accelerated due to radiation pressure. Therefore far from the nucleus only the nuclear sodium source can be detected.

The fast and slow peaks therefore represent two different neutral sodium tails: a narrow sodium tail produced by sodium released at or near the nucleus and a diffuse sodium tail that Cremonese and Fulle [1997] consider to have been released from dust. Cremonese and Fulle [1997] consider the diffuse sodium tail as explaining the results of Wilson et al. [1998] and consider the variability of the two sources to account for the difference between this and other observations.
Figure 2.9: Slit positions on April 23.9 UT used by Cremonese and Fulle [1997] to obtain measurements of neutral sodium intensities throughout the tail of comet Hale-Bopp. Slit positions are shown along the neutral sodium tail ($\beta = 82$) syn-dyne at 0.4, 0.89, 3.13, 5.07, 7.17 degrees from the nucleus.

By further analysis of the CoCam images taken by Cremonese et al. [1997b] (subtraction of the continuum image from the orange filter image), Cremonese and Fulle [1997] are also able to distinguish a diffuse neutral sodium tail coincident with the cometary dust tail observed at Hale-Bopp.

In Cremonese et al. [2002] and Cremonese [1999], the authors reviewed the current level of understanding of cometary sodium, focussing on the sodium tail observations of comet Hale-Bopp. They highlight the relative ease of obtaining sodium data with respect to data from other atoms, in particular noting that the availability of observations of the structure of neutral atom tails relies primarily on an instrument’s field of view and on the wavelength of the atomic emission [Cremonese et al., 2002].

Cremonese [1999] note that although several studies have tried to determine the source required to produce the sodium observed at comet Hale-Bopp, the results are inconclusive. The mechanism for neutral sodium atom release from parent molecules also remains unknown - potentially either photodissociation or photoionisation followed by dissociative electron recombination in the diffuse dust tail are reasonable candidates. The narrow sodium tail observed at Hale-Bopp was also discussed by Cremonese [1999]. The short lifetimes of the parent molecules calculated suggest that the sodium in this narrow tail may originate from sputtering on fresh surfaces of rapidly fragmenting dust, but again this result has not yet been proven [Cremonese, 1999].

In a later review paper, Cremonese et al. [2002] clearly indicate the need for successful models that explain sodium tail observations, particularly in understanding other processes operating in the coma. In creating a successful model Cremonese et al. [2002]
The Neutral Sodium Tail of Comet Hale-Bopp

(a) Profile obtained toward the dust tail, 0.4° from the nucleus. The slow component has a velocity of 6 km/s whereas the faster component has a velocity of 37.7 km/s [Cremonese and Fulle, 1997].

(b) Profile obtained towards fast sodium tail axis, 0.89° from the nucleus on identical spectrum to figure 2.10a but on opposite edge. The slow component has merged into the faster component, which has a velocity of 62 km/s. [Cremonese and Fulle, 1997].

Figure 2.10: Profile of sodium D lines of comet Hale-Bopp obtained on 23.9 April 1997. Neither spectra has been corrected by the comet velocity. F/S indicates the fast/slow neutral sodium tail emission components respectively.

hope that sodium measurements may be used to trace key processes in the coma (such as photodissociation, photoionisation, sputtering and dust production).

Furusho et al. [2005] report on a series of sequential spectroscopic observations of comet Hale-Bopp taken between September 1996 and May 1997 using the low-dispersion spectrograph (FBSPEC-1) on the 0.28 m Schmidt-Cassegrain telescope. During this time the development of the neutral sodium emission was monitored for the four months around perihelion. The setup has a resolution of about 10 Å, and covered around
Furusho et al. [2005] observed the region inside the central comet condensation (i.e. the inner coma), in order to avoid issues with increased continuum density in the jets seen in continuum images of comet Hale-Bopp prior to this date by West and Kidger [1997].

The analysis of Furusho et al. [2005] at comet Hale-Bopp was based on an approach presented by Watanabe et al. [2003] for comet 153P (Ikeya-Zhang). Watanabe et al. [2003] monitored neutral sodium from comet Ikeya-Zhang throughout its perihelion passage while it was between 0.511 AU and 0.764 AU. Watanabe et al. [2003] calculate the neutral sodium to dust flux ratio at comet Ikeya-Zhang in a small region 38".5 from the optocenter of the comet, for a range of heliocentric distances of the comet. Watanabe et al. [2003] suggest that if the neutral sodium was released from dust via photo-sputtering, the ratio of the rate of sodium production to the rate of dust production should be proportional to the incident solar flux, which varies with heliocentric distance, $R$, as $R^{-2}$. They find that this ratio varies as $R^{-5.1 \pm 1.0}$, which they state is too steep to be explained as a result of photo-sputtering and is likely to be the result of thermal desorption from cometary grains. Furusho et al. [2005] find a similar sodium to dust flux ratio of $R^{-5}$ or $R^{-6}$, which is consistent with the analysis of Watanabe et al. [2003]. However, both of these calculations rely on the spatial distribution of neutral sodium atoms being identical to that of dust in the region close to the comet observed by both studies, which may not be the case.

Consideration of the variation of the rate of neutral sodium production from dust via photosputtering with heliocentric distance should include both the variation of solar flux ($R^{-2}$) and the variation of the rate of dust production. The rate of dust production from the cometary nucleus varies with heliocentric distance as approximately $R^{-2.7}$ [Wilkening and Matthews, 1982]. For comet Hale-Bopp, Jewitt and Matthews [1999] find that the rate at which dust is released from the nucleus varies as $R^{-1.7}$ for $0.9 \leq R \geq 2.5$ AU. Therefore the rate of neutral sodium production from dust via photosputtering at comet Hale-Bopp at these heliocentric distances should be approximately proportional to $R^{-3.7}$.

Most authors have speculated that (based on modelling, theory and observation) the main sources of sodium in the neutral tail of Hale-Bopp were a nuclear (or near nuclear) source (possibly variable) and an extended dust source. Two separate sodium tails with different morphologies have been distinguished by some studies (one narrow and distinct from all other tails and one diffuse which was observed to overlap the dust tail, although in the Combi et al. [1997] data the diffuse tail appeared to coincide with the ion tail) but others have suggested that this primarily due to observation geometry. There is currently no consensus on the source(s) of sodium at Hale-Bopp, or at comets generally.

As previously stated Hale-Bopp was the dustiest comet observed to date at the time and this is likely to have affected the production of sodium. The overlap between the
ion and sodium tails observed by Combi et al. [1997] was apparently a coincidence, but it is surprising that similar results were not obtained by any other study despite taking observations on similar dates. Combi et al. [1997] initially suggested an ionic parent for sodium based on their observations of comet Halley and it seems likely that the primary source of sodium would depend on the environment present in the cometary coma. Therefore the balance of different sources of sodium at other comets may differ from that implied by the results of comet Hale-Bopp. Furthermore, most studies presented here highlight the need for more appropriate models of the processes required to produce a neutral cometary sodium tail.

2.6 Other Observations of Neutral Sodium Tails and Similar Features at Comets

Since the large number of studies of the neutral sodium tail of comet Hale-Bopp, neutral sodium tails and remarkably similar features have been observed at many other comets. In this chapter we review the literature relevant to observations of neutral cometary sodium tail-like features. The observations of neutral sodium tails at comets Hyakutake, NEAT and McNaught by the SOHO/LASCO instrument are considered in this thesis but have not been analysed quantitatively before despite their strong scientific value. These unanalysed LASCO datasets were gathered together for this study following private communication with Jones and Osborn [2015] and by use of the SOHO Science Archive [Osuna et al., 2010]. The neutral sodium tail at comet McNaught was analysed by Leblanc et al. [2008], and this work is therefore discussed in this chapter to provide a suitable background to the work we present in this thesis. The Schmidt et al. [2015] study of the neutral sodium emission of comet ISON is also discussed for background in this chapter, although comet ISON was observed by SOHO/LASCO no distinct neutral sodium tail was detected (most distinct neutral sodium tails are detected post-perihelion, but as comet ISON broke up around perihelion no neutral sodium tail was observed [Knight and Battams, 2014]) and therefore observations of comet ISON are not studied further in this thesis.

2.6.1 Sodium Observed in Near-Sun Comets

Near-Sun comets are comets that approach very close to the Sun with perihelia inside the orbit of Mercury at 0.307 AU (based on the convention adopted by Jones et al. [2016]). It is very difficult to study these objects from Earth when they are close to the Sun because they are typically many orders of magnitude less bright than the Sun. If a solar eclipse occurs coincidentally with the near-Sun comet’s perihelion it may still be observable, for example the eclipse comet (X/1882 P1) was observed in this manner [Vaquero and Vázquez, 2009].
As they approach very close to the Sun their surfaces are highly irradiated and all cometary material, including that which is typically considered refractory such as dust, may be sublimated. They are therefore extremely unlikely to survive perihelion passage unless they are initially very massive, and are often dynamically new objects on their first passage through the inner solar system (see chapter 1). Jones et al. [2016] present classification of different types of near-Sun comets based on a consideration of observable properties including:

- **Near-Sun Comet**: Any comet with a perihelion distance \( q \) less than the perihelion of Mercurys orbit \((0.307 \text{ AU} = 66 \text{ solar radii } (Rs))\).
- **Sunskirter**: \(3.45 \text{ Rs} < q < 30 \text{ Rs}\) (LASCO field of view)
- **Sungrazer**: \(1 \text{ Rs} < q < 3.45 \text{ Rs}\) (based on the fluid (strengthless) Roche Limit of the Sun, which is the point when solar tidal forces = comet’s internal gravity)
- **Sundiver**: \(q < 1 \text{ Rs}\)

The study of near-Sun comets has been revolutionised by the introduction of space based observatories, such as STEREO and SOHO, due to the difficulty inherent in performing such observations from Earth. At the time of writing this thesis 3168 near-Sun comets had been identified as a direct result of observations performed by the SOHO/LASCO instrument (see chapter 3.3 for more information of the instrument itself), with more being discovered on an almost daily basis [Battams, 2015]. A thorough review of the modern understanding of near-Sun comets, based primarily on the recent era of space-based observations, is presented in Jones et al. [2016].

Near-Sun comets may be dramatically different in appearance to comets such as Hale-Bopp because if dust is sublimated it will not form a distinct dust tail and if it is sufficiently close to the Sun the electrically-charged dust’s morphology is primarily dictated by the complex solar magnetic field rather than gravitational and radiation pressure effects, and therefore the appearance of ion tails may be strange. Indeed, the ion tail of comet C/2011 W3(Lovejoy) was observed by the Solar Dynamics Observatory (SDO) to trace out the highly structured solar magnetic field as it passed through the solar corona [Raymond et al., 2014].

Many near-Sun comets are members of the Kreutz group, that was studied extensively by Knight [2008]. Whether a near-Sun comet is a member of the Kreutz group or not is decided by its orbital parameters. Members of the Kreutz group are likely to have once been part of one parent body. The Kreutz parent body was probably weakened by the tidal forces and high intensity of solar radiation incident on the object at perihelion, which caused it to fragment into one or two larger bodies and a series of smaller objects that we now know as the members of the Kreutz group. No Kreutz group comets were detected by Knight [2008] SOHO observations after their perihelion passages, but comet Lovejoy (a member of the Kreutz group) survived after its perihelion in December 2011. Recently, comet C/2012 (ISON) was observed as a cloud of material post perihelion
with no indication of a condensed central nucleus. Sekanina and Kracht [2014] suggest that SOHO and STEREO observations of comet ISON are consistent with a rapid series of explosions occurring within the comet’s interior, which led to total fragmentation of the cometary nucleus approximately 3.5 hours prior to perihelion.

Unfortunately no distinct neutral sodium tail-like features were observed by solar observatories for comet ISON (preliminary analysis by Knight and Battams [2014], but the dramatic increase in intensity in the orange wavelengths of near-Sun comets has been attributed to neutral sodium emission by various authors (for example Biesecker et al. [2002] and Knight et al. [2010b]). Near-Sun comets observed by the inner coronagraph on SOHO/LASCO (C2) are typically very bright in the orange filter wavelengths, which has led to speculation that the features observed at these objects are neutral sodium. However, no spectroscopy can currently be performed close enough to the Sun to prove that this is the case.

Neutral Sodium at Comet C/2006 P1 (McNaught)  

Comet McNaught was first detected in 2006 by McNaught et al. [2006]. It had a perihelion distance of 0.171 AU, and so would be classified as a sunskirter using the Jones et al. [2016] convention. Snodgrass et al. [2008] used the European Southern Observatory Multi-Mode Instrument (EMMI) to perform imaging (broadband and narrowband) and spectroscopy (low resolution long slit and high resolution Echelle) of this comet in January and February 2008. Spectroscopy obtained by Snodgrass et al. [2008] on 29 January 2008 showed a strong sodium doublet emission and spatially asymmetric sodium D1 lines in the inner coma of comet McNaught. This strong neutral sodium emission was not present in spectra taken perpendicular to the tail, so Snodgrass et al. [2008] suggest that this may be an indication of a neutral sodium tail feature similar to that observed at comet Hale-Bopp but this characterisation would require further study.

Leblanc et al. [2008] also measured a sodium tail at comet McNaught using the THEMIS solar telescope, with the spectroscopic model of the telescope with one camera centred on the D2 emission line at 5889 Å with a band width of less than 6 Å. Unfortunately, Leblanc et al. [2008] were only able to take data on one day (10 January 2007), which was before the comet’s perihelion on 12 January 2007 at 12.8 UT, due to poor weather conditions. The observations of comet McNaught taken by Leblanc et al. [2008] differ from the Rauer et al. [1998] and Brown et al. [1998] observations of comet Hale-Bopp, as they measure the sunward peak as more intense than that observed at the nucleus.

Leblanc et al. [2008] compare the cometary sodium ejection rate between the value they measure at comet McNaught with that determined by different authors at comet Hale-Bopp. They extrapolate the values presented in the literature for the ejection of neutral sodium at comet Hale-Bopp to the heliocentric distance of their observation of comet McNaught (using the variation in solar photon flux as 1/r^2) and find their results
compare favourably with the extrapolated value when a correction is applied for comet McNaught being much dustier than comet Hale-Bopp (having a much higher dust \( A f \rho \)). Leblanc et al. [2008] assume that comets Hale-Bopp and McNaught are of similar compositions and that most of the sodium originates in cometary dust, and therefore find that the sodium production rate varies with solar photon flux. This seemingly indicates that the most likely dominant mechanism of release of neutral cometary sodium is via photo-sputtering, but they cannot rule out other mechanisms such as sputtering via cometary ions and solar wind ions. This result directly contradicts the study conducted by Furusho et al. [2005] at comet Hale-Bopp, where they found that the sodium production rate did not vary in the same manner as the variation in solar photon flux. This difference may indicate that the neutral sodium emission from comet McNaught had a different dominant source of sodium production to comet Hale-Bopp, or that the use of a flux to continuum ratio by Furusho et al. [2005] may vary unexpectedly due to dust production in concentrated jets within the coma of comet Hale-Bopp. Unlike Furusho et al. [2005], Leblanc et al. [2008] only study the neutral sodium emission from comet McNaught at one heliocentric distance.

Neutral Iron at Comet C/2006 P1 (McNaught)  
Other neutral atomic emissions have been seen at comets that are again thought to be a consequence of resonance fluorescence. Iron cometary spectral lines were first observed in 1882 [Brandt and Chapman, 2004] and clearly visible in spectra of comet Ikeya-Seki at 0.14 AU by Preston [1967]. It has been speculated that iron atoms should form a neutral iron tail (produced in the same manner as a neutral sodium tail, but with different resonant wavelengths).

A study by Fulle et al. [2007] in 2007 showed an additional tail at comet McNaught using the HI-1 wide field camera. On first glance the tail appeared to be similar to the neutral sodium tail first observed at comet Hale-Bopp by Cremonese et al. [1997b], but the spectral bandpass of the filter on STEREO HI-1 should not allow detection of the sodium doublet. There are two possible explanations of these phenomena: either the HI-1 bandpasses have changed since launch and now include the sodium D-line wavelengths or another neutral tail is responsible for these features that behaves similarly to neutral cometary sodium.

Fulle et al. [2007] found that the observed tail was consistent with a syndyne of \( \beta \approx 6 \), which does not support a dust tail hypothesis (for which a maximum \( \beta = 2 \) is more appropriate). They also found that the solar wind velocities calculated assuming an ion tail trapped in solar wind plasma are inconsistent with measurements obtained using NASA’s Advanced Composition Explorer by Davis and Harrison [2005]. Fulle et al. [2007] therefore considered a constant \( \beta \) that could account for variation in radiation pressure caused by variation in heliocentric velocity (based on the \( g \) factor). They calculated \( \beta \) for the thirteen most abundant chemical species in comets using solar ultra-violet flux, high resolution visible flux and the oscillator strengths of all resonant
lines (during quiet Sun conditions). Fulle et al. [2007] find that the predicted syndyne for iron based on this approach is consistent with observations, suggesting that a neutral iron tail is observed.

From calculations of the observed brightness of the tail Fulle et al. [2007] also find strong evidence against a dust tail hypothesis (graphite or fluffy grains). They calculate an ionisation lifetime for the species in the tail based on the brightness profile (and an inverse square relationship between lifetime and heliocentric distance), as approximately $\tau = (6.6 \pm 0.6) \times 10^5$ s at 1 AU. Fulle et al. [2007] then estimate the lifetime of each of the thirteen atoms they considered previously using theoretical cross sections and the same solar flux. Their calculated sodium ultra-violet photoionisation lifetime agrees with that observed by Cremonese et al. [1997b] for Hale-Bopp. From their results Fulle et al. [2007] suggest that the most appropriate species for the third tail observed at McNaught is iron, with a calculated lifetime of $\tau = 5.1 \times 10^5$ at 0.25 AU.

Although there has been no conclusive distinct neutral iron tail observation to date it remains a possibility that an iron tail (or the tails of other neutral species) may be observed at comets.

The Neutral Sodium Tail of Comet C/2012 S1 (ISON)  
Schmidt et al. [2015] imaged comet ISON during its perihelion passage on 19.5 UT November 2013 and 20.5 UT November 2013 using a small refracting telescope with a 7° field of view and narrowband filters centred at 5893 Å (sodium) and 6051 Å (dust continuum) with bandwidths of 14 Å and at the McDonald Observatory, which had previously been used to study the exosphere of planet Mercury.

Two datasets were analysed by Schmidt et al. [2015], on the two separate dates they were able to observe neutral sodium emission from comet ISON. Firstly bias, dark, flat-field and cosmic ray corrections were performed. Absolute calibration was obtained by Schmidt et al. [2015] using spectrophotometric standard stars and D line emission was isolated by subtracting dust continuum filtered images from sodium emission filtered images. Schmidt et al. [2015] also co-aligned frames by shifting them by the comet’s proper motion using data obtained from the JPL horizons database [Giorgini et al., 1996] and subtracted the median of approximately $10^4$ pixels in order to account for telluric sodium emission. Schmidt et al. [2015] then stacked the co-aligned, processed frames by their median value. The result of this processing is shown in figure 2.11.

The Schmidt et al. [2015] model of neutral sodium emission from comet ISON is discussed in more detail in chapter 4, but the comparison between their model on both dates and the observational data products is shown in figure 2.12. In order to facilitate comparison with the model, the data products were rotated to align with detector’s pixel rows, assuming that the tail was purely antisunward. To represent instrument aberration, Schmidt et al. [2015] also convolved the model result with a two dimensional
Other Observations of Neutral Sodium Tails and Similar Features at Comets

Figure 2.11: Data products from observations of neutral sodium emission at comet ISON on 19.5 November 2013 (top) and 20.5 November 2013 (bottom), reproduced from Schmidt et al. [2015]. Only two frames were stacked to produce the image on 19.5 November 2013, whereas ten frames were stacked to produce the image on 20.5 November 2013.

Gaussian with a width obtained from the point spread functions of nearby stars.

Schmidt et al. [2015] find that they are unable to reproduce the neutral sodium emission from comet ISON using their model with steady state conditions with a source close to the cometary nucleus. Their work suggests that approximately half of the neutral sodium production rate is due to extended dust sources, and is enhanced during the outburst. Schmidt et al. [2015] also note that the neutral sodium production rate they obtained for comet ISON, \((1.6 \pm 0.3) \times 10^{23}\) atoms/s on UT 19.5 Nov 2013 and \((5.8 \pm 1.0) \times 10^{23}\) atoms/s on UT 20.5 at a heliocentric distance of 0.44 AU (based on their model), was orders of magnitude smaller than that obtained by other authors for comet Hale-Bopp and McNaught, suggesting that the composition of comet ISON may have been very different from these comets.

Schmidt et al. [2015] predict that the neutral sodium tail of comet ISON would have become more extended after perihelion, as observed by Cremonese et al. [1997b], but unfortunately no measurements could be taken as Comet ISON’s disintegration was observed shortly after its perihelion by SOHO/LASCO and following that observation no central nucleus condensation could be detected.
2.6.2 Neutral Sodium Observed by the Rosetta Spacecraft

The Rosetta spacecraft has been orbiting the Sun in close proximity to comet 67P/Churyumov-Gerasimenko (67P) since August 2014 [Taylor et al., 2015]. It was designed to investigate the properties of the nucleus and surrounding environment of comet 67P [Glassmeier et al., 2007]. Previous cometary missions have greatly increased our understanding of the plasma processes relevant to comets, but have focussed on high activity comets, such as comet 1P/Halley [Carr et al., 2007]. The mission has been very successful to date and became the first mission to place a soft lander on the surface of a comet on 12th November 2014 [Ulandec et al., 2015]. Rosetta is also the first mission to follow a comet as its activity changes throughout its perihelion passage and consistently monitor surface changes at a comet in detail.

The Rosina experiment on board the Rosetta spacecraft was designed to study the neutral and ion environment surrounding comet 67P [Balsiger et al., 2007]. Using the Double Focussing Mass Spectrometer (DFMS, part of the Rosina experiment) Wurz et al. [2015] searched for sputtered refractory species when the comet was at approximately 3 AU. They detect neutral C, O, Na, K, Si, Ca, and S, in quantities that cannot reasonably be released by sublimation or from fragments of sublimation. Wurz et al. [2015] find an approximate anticorrelation between the origin maps of \(H_2O\) (released via sublimation) and neutral atoms (reproduced in figure 2.13), detecting neutral sodium in the winter hemisphere of the comet, which was considerably less active in \(H_2O\) than in
the summer hemisphere. Wurz et al. [2015] argue that these results are consistent with neutrals being sputtered from refractory particles on the surface of the comet nucleus by solar wind, which is damped by cometary activity (release of cometary material via sublimation). Schulz et al. [2015] also detected a high abundance of sodium in cometary dust grains collected by COSIMA (the COmetary Secondary Ion Mass Analyser) on board the Rosetta spacecraft beyond 3 AU.

Ellinger et al. [2015] note the issue in understanding the source of neutral cometary sodium in their study. Ellinger et al. [2015] do not consider observational data, but instead look at a chemical approach to understanding the origins of neutral cometary sodium. They speculate that the presence of neutral sodium within icy cometary material could indicate that nucleogenic heating was sufficient to melt the core of comets within the protosolar nebula, thereby washing sodium out of refractory cometary dust by roughly the same process that releases sodium from rocks on Earth. They also speculate that sodium within the icy matrix may be observed by the Rosetta spacecraft.

2.7 Summary

Many authors have studied neutral sodium in comets, particularly the neutral sodium tails produced by comet Hale-Bopp, but no consensus has emerged on the method of release of neutral sodium from cometary material, or even on the location from which it is released. There are five different mechanisms for neutral sodium production at
comets that are currently favoured: sputtering, photo-sputtering, thermal desorption, dissociative recombination, molecular dissociation from parents with long dissociation lifetimes and release of neutral sodium resulting from collisions between dust particles. The distributions in space and velocity caused by each of these mechanisms is not well determined for the cometary environment in general, and all mechanisms have not yet been considered in detail by one author for any particular comet.

Before comet Hale-Bopp, relatively little was known about neutral sodium in comets and most of the data came from spectroscopy and therefore only considered neutral sodium emission very close to the cometary nucleus. Oppenheimer [1980] noted that at the heliocentric distances sodium had been observed meant that it could not be sublimated from dust, as temperatures were insufficiently high.

Most work on neutral cometary sodium has studied features in the observations of comet Hale-Bopp, following the initial detection in spectra by Kawabata and Ayani [1997] and the detection of a distinct neutral sodium tail by Cremonese et al. [1997b]. Cremonese et al. [1997b] determined that the tail they observed strongly in the orange filter using CoCam must be the result of neutral sodium atom emission using a simple Finson and Probst [1968] model.

Many authors have commented on the coincidence of the neutral sodium tails they have observed with another cometary tail feature, either the dust tail (e.g. Wilson et al. [1998], Rauer et al. [1998], Cremonese et al. [1997b]) or the ion tail (e.g. Combi et al. [1997]). This approach is insufficient to understand neutral sodium because of the unintuitive nature of the resonance fluorescence that determines the tail’s morphology, but does provide a good starting point for models.

Although simple scaling arguments, such as that presented by Ip and Jorda [1998], provide a good step for initial analysis, they are insufficient to fully characterise the variable environment surrounding a comet. Two neutral sodium tails were observed at comet Hale-Bopp by Cremonese et al. [1997b] and Kawakita and Fujii [1998]: one diffuse and one narrow. Barker et al. [1997] suggest that the narrow neutral sodium feature is the result of sodium released from the nucleus directly, whereas the diffuse sodium tail is the result of sodium released in situ in the dust tail. All authors whose works are discussed in this chapter agree that source of neutral sodium based at the cometary nucleus is likely, but disagree on its significance.

Combi et al. [1997] suggest that neutral sodium is likely to originate in two separate, variable sources: one near the nucleus and one in the plasma tail. Cometary ions are picked up by interplanetary magnetic field frozen into the solar wind and accelerated to form a distinct ion tail. Therefore cometary sodium produced by dissociative recombination would likely originate in the high velocity ion tail. Ip and Axford [1986] also suggest that dissociative recombination may be a source of loss of neutral cometary sodium in regions of high $H_2O$ density, which may explain why the decrease of neutral
sodium emission close to the cometary nucleus follows $1/r$, but further away shows a more extended source. However, the results of Brown et al. [1998] suggest that a neutral sodium source in the ion tail is unlikely as their observations could not be successfully reproduced by a model which used a neutral sodium tail source centred on the ion tail with ion tail velocities. Due to this, that the velocities involved in the neutral sodium tail and that the neutral sodium tail observed by Cremonese et al. [1997b] was distinct, we do not consider a source in the ion tail to be likely but it cannot be ruled out conclusively by any of these studies.

As it is not possible to determine the spatial location of the source of the neutral sodium tail conclusively, determination of the mechanism which produced the neutral sodium tail(s) observed at comet Hale-Bopp is currently impossible. The mechanisms favoured by each of the authors whose works are discussed in this chapter for the release of neutral cometary sodium is given in table 2.3, in the order they were reviewed. Inclusion of observational effects in an orbital model may allow extraction of the origin of the source of neutral sodium in comet Hale-Bopp and may therefore provide the first step to understanding the mechanisms which released neutral sodium from this comet and whether they are variable.

The brightening of near-Sun comets due to vaporisation of dust containing sodium had been discovered before comet Hale-Bopp [Huebner, 1970], but the availability of technology capable of studying near-Sun comets as they approach very close to the solar surface, such as the LASCO coronagraph on SOHO and the THEMIS telescope, have greatly increased the ability for new comets to be detected and studied. This has been very advantageous for the study of neutral sodium at near-Sun comets, but the production mechanisms for these comets may be very different to those where neutral sodium had previously been observed as it may be possible to sublimate cometary sodium atoms in some cases. It is likely that other mechanisms result in neutral sodium release from near-Sun comets, particularly when they are close to the Sun.

Neutral sodium emission has been detected in near-Sun comets McNaught [Snodgrass et al., 2008; Leblanc et al., 2008] and ISON [Schmidt et al., 2015]. The result of Leblanc et al. [2008] contradicts the study of Furusho et al. [2005] and finds that photosputtering is the dominant process of sodium release in the cometary environment based on simple scaling arguments between the rate of neutral sodium production at comets McNaught and Hale-Bopp, which may not be appropriate. Schmidt et al. [2015] produce a model that agrees with the Brown et al. [1998] model, and find that roughly half of the neutral sodium is released from the nucleus and half is released from extended dust sources.

In situ observations of neutral cometary sodium have the potential to assist in understanding ground-based observations of neutral sodium emission, that could help improve the understanding of the cause of neutral sodium emission in the cometary environment. The Rosetta mission to comet 67P/Churyumov-Gerasimenko is providing new insight into the development of cometary features at a low activity comet, but
these objects typically do not display significant neutral sodium tail features. However, the results of the Rosetta mission have so far led to the identification of neutral sodium sputtered from the cometary nucleus by Wurz et al. [2015] and the detection of neutral sodium within cometary dust grains by Schulz et al. [2015]. Ellinger et al. [2015] also speculate that Rosetta has the potential to identify plasma sources of neutral sodium that could indicate nucleogenic heating within cometary nuclei in the protosolar nebula.

The primary issue in this field of research is that some of the initial information surrounding the production of neutral cometary sodium is lost due to the rapid, resonant acceleration of the neutral sodium atoms by the Swings and Greenstein effects. The neutral sodium motion resulting from these effects is unintuitive and therefore the first step in determining the mechanism(s) of neutral sodium production in comets must be to determine the origin of cometary sodium by understanding which features are a direct result of the physical, Doppler-shift related effects at the comet (and the observational geometry) and which features are the result of a particular production mechanism. This is the principle aim of this thesis. It is important to note that different comets may have different dominant neutral sodium production mechanisms, as they have different compositions and perihelia.
<table>
<thead>
<tr>
<th>Date</th>
<th>Type of Data</th>
<th>Feature(s) Observed</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 March and 5 April 1997</td>
<td>Spectroscopy</td>
<td>Na close to nucleus (between the fields of view of Cremonese et al. [1997b] and Arpigny et al. [1998])</td>
<td>Barker et al. [1997]</td>
</tr>
<tr>
<td>14 March, 16 April 1997</td>
<td>Spectroscopy</td>
<td>Na close to nucleus</td>
<td>Rauer et al. [1998]</td>
</tr>
<tr>
<td>17, 20 March 1997</td>
<td>Wide Field Narrowband Filtered Imaging</td>
<td>Diffuse NST, no narrow NST</td>
<td>Wilson et al. [1998]</td>
</tr>
<tr>
<td>17 March, 19 April 1997</td>
<td>Spectroscopy</td>
<td>Na close to nucleus. Before perihelion: diffuse NST, no narrow NST. After perihelion: Diffuse NST and narrow NST (stated that this was due to $g$ factor variation, not change in production rate of one source).</td>
<td>Kawakita and Fujii [1998]</td>
</tr>
<tr>
<td>25-27 March and 15-17 April 1997</td>
<td>Spectroscopy</td>
<td>Na close to nucleus</td>
<td>Arpigny et al. [1998]</td>
</tr>
<tr>
<td>8, 10 April 1997</td>
<td>Spectroscopy</td>
<td>Na close to nucleus</td>
<td>Brown et al. [1998]</td>
</tr>
<tr>
<td>16-22 April 1997</td>
<td>Wide Field Narrowband Filtered Imaging</td>
<td>Narrow NST</td>
<td>Cremonese et al. [1997a]</td>
</tr>
<tr>
<td>19, 20, 23 April 1997</td>
<td>Spectroscopy</td>
<td>Na close to nucleus</td>
<td>Cremonese et al. [1997b]</td>
</tr>
<tr>
<td>19 April 1997</td>
<td>Spectrographic Images $10^4$km and $10^6$km from the comet nucleus.</td>
<td>Diffuse NST, no narrow NST</td>
<td>Kupperman et al. [1998]</td>
</tr>
<tr>
<td>Various, between Septem-ber 1996 - May 1997</td>
<td>Spectroscopy</td>
<td>Na close to nucleus</td>
<td>Furusho et al. [2005]</td>
</tr>
</tbody>
</table>

Table 2.2: List of observations of comet Hale-Bopp discussed in this chapter, including observations of sodium close to the nucleus and the neutral sodium tail (NST). Comet Hale-Bopp’s perihelion occurred on 1 April 1997.
<table>
<thead>
<tr>
<th>Reference</th>
<th>Location of sodium release</th>
<th>Mechanism of sodium release</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cremonese et al. [1997b]</td>
<td>At or Near Nucleus</td>
<td>-</td>
</tr>
<tr>
<td>Wilson et al. [1998]</td>
<td>Extended Source Tailward</td>
<td>Release from dust grains</td>
</tr>
<tr>
<td>Combi et al. [1997]</td>
<td>Ion Tail</td>
<td>Dissociative Recombination</td>
</tr>
<tr>
<td>Rauer et al. [1998]</td>
<td>Extended source</td>
<td>Sublimation from nucleus or dust particles, sputtering from dust grains, or second generation species (more complex mechanism)</td>
</tr>
<tr>
<td>Ip and Jorda [1998]</td>
<td>-</td>
<td>Collisions between very small grains</td>
</tr>
<tr>
<td>Arpigny et al. [1998]</td>
<td>Nucleus source and extended source</td>
<td>-</td>
</tr>
<tr>
<td>Barker et al. [1997]</td>
<td>Nucleus source and extended source (from dust)</td>
<td>-</td>
</tr>
<tr>
<td>Kupperman et al. [1998]</td>
<td>-</td>
<td>Photodissociation of NaOH</td>
</tr>
<tr>
<td>Brown et al. [1998]</td>
<td>Nucleus source and extended source</td>
<td>-</td>
</tr>
<tr>
<td>Kawakita and Fujii [1998]</td>
<td>Nucleus source</td>
<td>-</td>
</tr>
<tr>
<td>Cremonese and Fulle [1997]</td>
<td>Nucleus source and extended source (from dust)</td>
<td>Nucleus source release due to molecular process e.g. dissociation</td>
</tr>
<tr>
<td>Furusho et al. [2005]</td>
<td>-</td>
<td>Thermal desorption from cometary grains</td>
</tr>
</tbody>
</table>

Table 2.3: Summary of mechanisms and source locations for cometary sodium release at comet Hale-Bopp discussed in this review.
Chapter 3

Instrumentation

In this chapter we discuss the general approach used to observe cometary sodium (chapter 3.1) and the specific instrumentation used to produce the observations used for comparison with the neutral sodium tail model we have developed (chapters 3.2 and 3.3).

3.1 Introduction

To be able to successfully interpret neutral sodium tail observations the method, geometry and physics of the observation must be understood in detail. This is most effectively established through the comparison of processed observations with a fully heliocentric distance and velocity dependent orbital neutral sodium tail model, such as that presented in chapter 5.

There are many different instruments capable of characterising neutral cometary sodium emission and each provides insight into the morphology and structure of the neutral cometary sodium tail. A combination of the general approaches discussed in this chapter provides the most complete data set on the morphology and structure of the tail, but due to time constraints, instrument availability and the position of the observatory it may not always be possible to study the variability of the tail. The small number of recent concentrated cometary observation campaigns use networks of observatories (both professional and amateur) to overcome these issues, but many resources are required to successfully manage this approach and it may not always be practical.

Ground/Space Based Observatories  Recording infra-red or ultra-violet emissions usually requires space based measurements (due to absorptions in the Earth’s atmosphere), but as the sodium D line emission is in the visible spectral range either ground or space based approaches are appropriate. Historically it has been difficult to perform ground based sodium observations, as sodium is also present in the atmosphere
Ground-based observing platforms relevant to this thesis in the study of comet C/1995 O1 (Hale-Bopp)

of the Earth [Cremonese, 1999]. Observers therefore need to be able to identify the telluric sodium emission in their data and effectively remove it from their data. In most cases this remains preferable to the large costs involved in recording space based measurements. A background telluric sodium sky image may be subtracted for wide field imaging but for low resolution spectroscopy the cometary sodium emission is likely to be difficult to extract when a comet does not have sufficient relative radial velocity with respect to the Earth, as in this case telluric sodium emission lines and the cometary sodium emission lines are not sufficiently distinct.

**Wide Field Imaging** Wide field imaging of comets allows many different regions to be observed simultaneously. This is particularly useful in characterising cometary tails if the tails do not overlap, but can also allow the overall morphology of a neutral sodium tail observed to be established when appropriate filters are available in the relevant emission bands (assuming no other cometary species emit significantly in that band and the bandpass of the filter is relatively narrow, which is the case for neutral sodium emission). Neutral sodium has been studied extensively in planetary atmospheres, the interstellar medium and stellar envelopes. Therefore in general observatories already have the appropriate interference filter required to produce wide field images of cometary sodium [Cremonese et al., 2002]. Wide field images are one of the easiest ways to detect a sodium tail, although they do not provide the velocity information that can be deduced from relevant spectra of the same phenomenon.

**Spectroscopy** Spectra can play a significant role in characterising cometary emissions, particularly if several spectra are taken at different slit positions throughout the tail and coma (for example figure 3.1). In the case of sodium emission, high resolution spectra are used primarily to calculate the velocities of sodium atoms in the slit region, which can be important in determining the validity of theoretical models because the Doppler shift of a neutral cometary sodium atom directly determines the intensity of its emission (see chapter 2.2 for more details). Spectroscopy can also provide valuable information about the velocity distribution of neutral cometary sodium emission on a very small scale, very close to the nucleus.

### 3.2 Ground-based observing platforms relevant to this thesis in the study of comet C/1995 O1 (Hale-Bopp)

The instruments used by Cremonese et al. [1997b], Brown et al. [1998] and Rauer et al. [1998] in the relevant studies of comet Hale-Bopp (see chapter 2 for more details) are discussed in detail in this chapter to provide the necessary context for the interpretation of the comparison between the observations and COMPASS simulation results presented in chapter 6.
Ground-based observing platforms relevant to this thesis in the study of comet C/1995 O1 (Hale-Bopp)

3.2.1 Imaging

The Comet Camera, CoCAM, was developed at the Isaac Newton Group in La Palma and used by Cremonese et al. [1997b] to obtain high quality, ground based wide field images of comet Hale-Bopp [Pollaco et al., 2013]. It is no longer in use. CoCAM had a large field of view (maximum width of approximately 20°), which allowed it to image both the coma and tails simultaneously [Pollaco et al., 2013]. A variety of different filters were used in conjunction with CoCAM to investigate different aspects of cometary physics. Those relevant to the study of cometary sodium tails are listed in table 3.1, but others were used for other studies, such as CN.

The CoCAM instrument itself consisted of a standard set of camera lenses, which imaged onto a cryogenically cooled, EEV CCD detector (2000x1000 pixels). Images were collected using a standard ING CCD controller, downloaded onto a dedicated SUN Sparc computer system, scientifically processed and made available to the scientific community via a website, Pollaco et al. [2013], that is still available. A photograph of the instrument is shown in figure 3.2.

<table>
<thead>
<tr>
<th>Filter</th>
<th>Central Wavelength (Å)</th>
<th>Full Width Half Maximum (Å)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Solar Continuum (Dust scattering)</td>
<td>6250</td>
<td>25</td>
</tr>
<tr>
<td>Sodium</td>
<td>5892</td>
<td>15</td>
</tr>
<tr>
<td>Ion ($H_2O^+$)</td>
<td>6185</td>
<td>42</td>
</tr>
</tbody>
</table>

Table 3.1: Table showing some of the filters used in conjunction with the CoCAM wide field imaging instrument Cremonese et al. [1997b].

3.2.2 Spectroscopy

A spectrograph typically consists of an entrance slit, a collimator to produce a parallel beam of light, a grating to separate out the desired wavelength range and a camera
Ground-based observing platforms relevant to this thesis in the study of comet C/1995 O1 (Hale-Bopp)

Figure 3.2: A photograph showing the relatively simple construction of the CoCam instrument used to take wide field images comet Hale-Bopp. Image reproduced from Pollaco et al. [2013].

and detector to focus and record the result. The grating (either transmission or more commonly reflection) acts like interference from multiple slits, with the resultant interference pattern described by Jenkins and White [1957]:

\[ d(sin \phi + sin \theta) = m \lambda, \]  

where \( d \) is the slit separation, the light is incident on the grating at an angle \( \phi \), \( \theta \) is the angle at which the order is formed, \( m \) is the order of the maxima and \( \lambda \) is the incident wavelength of the light. Differentiating this equation also gives a relation for the angular dispersion of the spectrograph (i.e. the separation of any two wavelengths \( \lambda_1 \) and \( \lambda_2 \)):

\[ \frac{\delta \theta}{\delta \lambda} = \frac{m}{d \cos(\theta)}, \]  

which is typically quoted when considering its performance. A high resolution Echelle spectrometer also includes a cross disperser to separate the wavelength order desired for the measurements. Three spectroscopic instruments were used by Brown et al. [1998] and Rauer et al. [1998] to obtain the neutral sodium tail measurements of comet Hale-Bopp modelled in this thesis. They are:

- Lick Observatory 0.6 m coudé auxiliary telescope coupled to the Hamilton Echelle Spectrometer (used by Brown et al. [1998]).
- Observatoire de Haute-Provence CARELEC Spectrograph on the 1.93 m telescope (used by Rauer et al. [1998]).
• William Herschel Telescope, ISIS Double Beam Spectrograph (used by Rauer et al. [1998]).

The Lick Observatory 0.6 m Coudé auxiliary telescope coupled to the Hamilton Echelle Spectrometer was first used in 1986 and is described in detail by Vogt [1988]. A diagram of the optical design of the instrument is shown in figure 3.3 from the top and side. The instrument includes an Echelle spectrometer, which includes an Echelle diffraction grating to produce high resolution spectra and a prism to select the order desired. An Echelle grating has a relatively coarse spacing of grooves, but are typically blazed, meaning that the grating has a steep sawtooth profile. The blaze of the grating must be optimised for the wavelength chosen. The Hamilton Echelle Spectrometer was initially designed for use in high resolution stellar spectroscopy, and so was different from the traditional design of an Echelle spectrometer in that it has a relatively large collimated beam size, uses prisms instead of gratings for cross dispersion (order separation) and includes a fast (f/1.67) folded Schmidt camera.

![Figure 3.3](image)

Figure 3.3: A diagram of the layout of the Hamilton Echelle Spectrometer, reproduced from Vogt [1988].

The Observatoire de Haute-Provence CARELEC spectrograph on the 1.93 m telescope
Space based remote observing platforms relevant to this thesis in the study of near-Sun comets: SOHO/LASCO

is described in detail by Lemaitre et al. [1990]. A diagram of the optical design of the CARELEC long slit spectrograph is shown in figure 3.4.

Figure 3.4: A diagram of the CARELEC spectrograph on the 1.93 m telescope at the Observatoire de Haute-Provence during the perihelion passage of comet Hale-Bopp in 1997, reproduced from Lemaitre et al. [1990].

The ISIS double beam spectrograph at the 4.2 m William-Herschell Telescope (WHT) was used by Rauer et al. [1998] to complement the other observations they had taken of comet Hale-Bopp. Each of the two arms of ISIS (red and blue) may be considered as conventional spectrographs, where the components have been optimised for either the red or blue wavelength range.

3.3 Space based remote observing platforms relevant to this thesis in the study of near-Sun comets: SOHO/LASCO

The SOlar Heliospheric Observatory (SOHO) spacecraft was launched in 1995. Its primary objective was to study the internal structure of the Sun, heating effects in the solar corona and the production and acceleration of the solar wind [NASA, 2013]. However, its operation has also resulted in an enormous increase in the number of sun-grazing comets detected [Knight, 2008].

SOHO is composed of twelve instruments, of which LASCO, the Large Angle and Spectrometric Coronagraph, has arguably been the most significant to the study of cometary physics. A detailed description of the instrument is given by Brueckner et al. [1995]. LASCO consists of three telescopes (C1, C2 and C3) that each image
Space based remote observing platforms relevant to this thesis in the study of near-Sun comets: SOHO/LASCO

an area further from the Sun than the last, between 1.1-30 solar radii. Coronagraphs typically suffer from a degradation of the image close to the edge of the field of view, therefore the fields of view partially overlap to overcome this problem. Each of the three telescopes has a filter wheel, polariser wheel, shutter and a 1024-1024 pixel CCD. C1 has a narrow passband Fabry-Perot interferometer that is tuned to hot coronal emission lines, and as a result is unlikely to detect cometary emission [Biesecker et al., 2002]. Indeed, no comets have been detected by C1 (and it ceased operations in 1998), so it is not considered further in this work [Knight, 2008]. The C2 and C3 coronagraphs are externally occulted instruments, which image annular fields of view from 1.5-6 solar radii and 3.7-30 solar radii respectively [Brueckner et al., 1995]. A diagram of the C2 and C3 LASCO instruments, showing the external occulting disk, internal occulter and Lyot stop, is given in figure 3.5. The internal occulter, field stop, Lyot stop and baffles are used to reduce stray light within the telescope to allow a clearer image of the corona to be produced.

Figure 3.5: Diagrams of the LASCO C2 (left) and C3 (right) instruments on the SOHO spacecraft, reproduced from Brueckner et al. [1995].

As they image different regions of the corona, they are optimised to work in different brightness ranges: C2 and C3 in $2 \times 10^{-7} - 5 \times 10^{-10} B_\odot$ and $2 \times 10^{-7} - 5 \times 10^{-10} B_\odot$ [Brueckner et al., 1995]. The units of disk mean solar brightness, $B_\odot$, are the physical unit traditionally used for coronagraphic data, and are the units used for calibrated (level 1) LASCO images. These units are used because coronagraphs are designed to measure the scattering of sunlight by electrons in the corona, with the signal integrated over the line of sight. When cometary emission is observed by a coronagraph, the emission from the comet has also been scattered by the electrons within the corona.

The majority of Kreutz sungrazing comets detected by LASCO have been seen using the C2 telescope, but for our purposes the C3 instrument is more significant as the
increased field of view and greater distance from the Sun (leading to weaker coronal emission) increases the probability of distinct neutral sodium tails being observed. The three C3 filters most important for the study of sodium in comets are:

1. Orange filter - strongly shows sodium emission and dust continuum emission.
2. Blue filter - strongly shows the emission characteristic of an ion tail and dust continuum emission.
3. Clear filter - shows all emission in range (containing blue and orange filter wavelengths).

The response curves for all filters available on SOHO/LASCO C3 are given in figure 3.6. It shows that clear filter contains the spectral bands of the blue and orange filter and that there is only a narrow overlap between the spectral bands of the blue and orange filters.

The LASCO instrument has been very successful in observing near-Sun comets, but as the primary observation target was the corona, observing comets using LASCO introduces some challenges. The features of interest in comets cover a very wide range in brightness, so when operating LASCO a choice must sometimes be made between observing the bright cometary nucleus or fainter cometary features, such as tails and disconnection events. The LASCO instrument team choose the exposure lengths based on available brightness estimates, sometimes before the comet is in the field of view. Constructing appropriate estimates is challenging so occasionally bright near-Sun comets are seen to saturate the detector. This will typically result in a saturation spike at the cometary nucleus, as the overabundance of charge in the CCD will bleed into other pixels along the same row. The overabundance of charge primarily bleeds along the same row.

Figure 3.6: SOHO/LASCO C3 Filter Response Curves [NAVY, 2016].
row as the extremely bright pixel, because the charge leaks easier along the direction in which the CCD image is read out by the associated electronics. Similar saturation spikes are also often observed when a planet, such as Mercury, is visible in the LASCO field of view. An example showing saturation spikes observed by LASCO is shown in figure 3.7.

Figure 3.7: LASCO composite image showing planets Mercury, Saturn, Jupiter and Venus (from left to right), reproduced from Hill [2016]. Saturation spikes are clearly visible for all planets, and are produced by objects in the LASCO field of view that are extremely bright. Note that all the saturation spikes lie along the same row, because the charge leaks easier along the direction in which the CCD is read.

LASCO C3 images are available publicly on the SOHO website [NASA, 2013] in their uncalibrated ‘level-0.5’ form. Level-0.5 images have been processed from the original spacecraft data into rectified FITS files with solar north ‘up’ [Morrill et al., 2006]. Level 0.5 images may then be calibrated using the IDL Solarsoft routines for SOHO, that were developed by the LASCO team [Freeland and Handy, 1998]. Calibrated images are known as Level 1 images and have undergone the following processing, as described by Morrill et al. [2006]:

1. Offset bias subtraction (to remove positive voltage applied to the CCD to ensure it does not read a negative value).
2. Exposure correction factor multiplication (to correct for the fact that the true exposure time is slightly different from the exposure time recorded in the header).
3. Extrapolation to replace missing blocks of data.
4. Calibration of image from number of counts to disk mean solar brightness. The calibration factor used for the orange filter on LASCO C3 with a clear polariser is $0.0286 \left(10^{-10} B/B_\odot\right)/(DN/pixel \ second)$.
5. Multiplication by vignetting function (to correct for the reduction in light received at the CCD due to the optics of the telescope). The vignetting in C3 changed slightly due to a change in the optics of the telescope during the mission interrupt in 1998, therefore vignetting functions pre- and post- interrupt are used for C3.

7. Application of correction for geometric distortion.

8. Multiplication by distortion corrected mask containing the occulter, pylon and outer edge of the coronagraph.

9. Correction for spacecraft roll (to orient solar north vertically upwards in image).

The processed LASCO C3 level-1 images are used in our analysis.
Chapter 4

Previous Approaches to Modelling Cometary Neutrals

Modern computational modelling techniques have been invaluable to the understanding of cometary observations and have also allowed theories of cometary processes to be tested rigorously by enabling future predictions of the features expected at given comets. In this chapter we present a brief introduction the approaches used by different authors to model neutral sodium emission in comets. We first present a brief introduction to the Haser [1957] model. The Haser [1957] model does not provide information on the emission from neutral cometary material, but it is the model on which most cometary neutral outflow models are based and therefore provides important context for the other models used to model neutral sodium emission and background to the choice of source distributions in COMPASS (see chapter 5). All neutral sodium tail models discussed here concern the tail observed at comet Hale-Bopp, except for the final model that was created by Schmidt et al. [2015] for comet ISON and was originally developed to understand the neutral sodium tail observed at planet Mercury.

4.1 Modelling the Outflow of Neutral Cometary Gas

The Haser [1957] model is often used to estimate the gas production rate at a comet. It is based on a number of assumptions:

- Outgassing is isotropic and the comet nucleus is assumed to be spherical.
- Gas streams out of nucleus at constant velocity.
- Parent species at the nucleus decay directly into the species observed with a scale length of $l_p$, which themselves decay into new species with a scale length of $l_d$.

Under these assumptions the number of particles in a given distance from the nucleus, $n$, can be described by the Haser [1957] model as:
\[ n(r) = \frac{Q}{4\pi v_{\text{out}} r^2} \left( \frac{l_d}{l_p - l_d} \right) \left( e^{-r_n/l_p} - e^{-r_n/l_d} \right), \]  

(4.1)

where \( Q \) is the production rate, \( v_{\text{out}} \) is the gas outflow velocity, \( r \) is the cometocentric distance, and \( r_n = r - r_n \) where \( r_n \) is the radius of the cometary nucleus. Making the assumption that the nucleus can be approximated as a point source and that \( l_p << l_d \), this may be simplified to:

\[ n(r) = \frac{Q}{4\pi v_{\text{out}} r^2} \left( e^{-r/l_d} \right). \]  

(4.2)

This can be further simplified by assuming the daughter species is produced directly from the parent and expands from the nucleus at a constant speed at sublimation, meaning that the scale length is given by:

\[ l_d = \tau v_{\text{out}}, \]  

(4.3)

where \( \tau \) is the lifetime against destruction, which for the case of neutral sodium in the coma emitted directly from the nucleus may be approximated as the lifetime against photoionisation, so equation (4.2) may be written as:

\[ n(r) = \frac{Q}{4\pi v_{\text{out}} r^2} \left( e^{-r/l_d} \right). \]  

(4.4)

This may be further simplified by assuming the lifetime of the daughter molecule is large as:

\[ n(r) = \frac{Q}{4\pi v_{\text{out}} r^2}, \]  

(4.5)

which is the form used in one of the COMPASS source distributions (see chapter 5 for more details).

### 4.2 Modelling Neutral Cometary Sodium

Although ion and dust tails remain the most studied cometary features to date, when a comet is extremely active other features become evident. Neutral tails were speculated to form in these situations but were not imaged until a neutral sodium tail was detected during the 1997 apparition of comet Hale-Bopp by Cremonese et al. [1997b].

Historically sodium tails were characterised using the syndyne model, with \( \beta = 82 \pm 3 \) for cometary sodium Cremonese [1999]. However this parametrisation does not fully
characterise the motion of sodium in comets, due to its highly efficient resonance fluorescence (see chapter 2.2), and the sensitivity of this efficiency to the heliocentric velocity of the atoms.

Cremonese and Fulle [1997] use Keplerian mechanics based on the Finson and Probstein [1968] model to estimate the position of the neutral sodium tail. The Finson and Probstein [1968] model is discussed in more detail in chapter 8, where it is used in conjunction with COMPASS to generate a dust tail source for neutral cometary sodium release. Cremonese and Fulle [1997] establish an equation for the $\beta$ (defined in equation (1.1)) of the dust particles:

$$\beta(\text{Na}) = \frac{hg(L)(1\text{AU})^2}{\lambda GM_S M_{\text{Na}}},$$

(4.6)

where $g(L)$ is the g factor at 1 AU (which varies approximately as a function of the distance down the tail, $L$, because the heliocentric velocity varies down the tail), $(1 \text{AU})^2$ encompasses the variation in the g-factor with heliocentric distance, $h$ is Planck’s constant, $G$ is the gravitational constant, $M_S$ is the mass of the Sun and $M_{\text{Na}}$ is the mass of the sodium atom. This follows from the basic definition of $\beta$ as the ratio between the radiation pressure incident on the particle, given by:

$$F_{\text{rad}} = \frac{hg}{\lambda},$$

(4.7)

as the radiation pressure force is the result of momentum transfer from the photons to the particles (photons have no mass so their momentum, $p$, is given by $p = E/c = h/\lambda$ where $E$ is the energy of the photon, $\lambda$ is its wavelength and $h$ is Planck’s constant), and the gravitational force acting on the particle, given by Newton’s law of gravitation:

$$F_{\text{grav}} = \frac{M_S M_{\text{Na}} G}{R^2},$$

(4.8)

where $R$ is the comet’s heliocentric distance. Equation (4.6) is an approximation because it does not take into account the initial velocity of the sodium atom and assumes all sodium atoms are produced from a point source at the comet nucleus. Cremonese and Fulle [1997] found that a constant $\beta = 82 \pm 3$ was most appropriate for narrow sodium tail they observed. The results of the Cremonese et al. [1997b] model are shown in figure 4.1. The principal achievement of this model was to show that the theoretical photoionisation lifetime of approximately 2 days at 1 AU is far better at characterising the intensity distribution along the tail if the assumptions made in this model are accurate.

Combi et al. [1997] studied the extent of the sodium tail at Hale-Bopp using a model based on the heavy species hybrid gasdynamic/Monte Carlo calculation presented in
Figure 4.1: Parameters used as a function of tail distance reprojected along the antisolar direction to investigate the neutral sodium tail at comet Hale-Bopp by Cremonese et al. [1997b]. Top left: Theoretical g-factors for the D1 line (bottom), D2 line (middle), and both combined (top). Top right: $\beta$ values resulting from use of combined g-factor based on computed velocity curve shown in the lower left plot. Bottom left: Measured velocities deprojected along the antisolar direction (points), compared with the computed velocity distribution (curve). Bottom right: Observed brightness distribution in the tail as measured from the high-resolution spectra vs. model predictions for two photoionization lifetimes, assuming an Na lifetime at 1 AU of $\tau = 14$ hours and $\tau = 47$ hours (theoretical lifetime adopted by most comet studies).

Combi and Fink [1993] and Smyth et al. [1995], that had previously been used to explain observations of OH and NH$_2$ at comet Halley. The model considers a nucleus at a fixed heliocentric distance and could account for collisions between sodium atoms and background coma gas (specified by a hydrodynamic description of the outflow). They use the cross section of sodium-water collisions as a parameter (as it was not available in literature).

In order to accurately model the sodium distribution Combi et al. [1997] included heliocentric velocity dependent radiation pressure acceleration and resonance fluorescence. Their approach combines the resonant fluorescence g factors of both lines in the sodium D doublet to calculate the resulting radiation pressure acceleration as a function of heliocentric velocity (shown in figure 4.2). Both the Swings and Greenstein effects are treated identically in this model.

In their model sodium is produced at or near the nucleus (a point source) and is initially collisionally entrained in (and in equilibrium with) the outflowing gas, until it reaches
the collision radius. The collision radius is defined as the distance where the mean free path of sodium atoms equals the distance to the nucleus. Inside the collision radius sodium atoms in the model experience both radiation pressure and collisional forces, outside they experience only radiation pressure.

Once the atoms reach the collision radius they are released with a random local velocity (based on the small thermal spread given by their hydrodynamic temperature). The trajectories of individual atoms are then calculated using the integration method described in the studies of Combi and Smyth [1988] and Combi and Fink [1993]. 500,000 atoms are considered in each simulation.

The Combi et al. [1997] model showed that a nucleus source alone could not be responsible for the flattened tailward distribution observed at Hale-Bopp. Before this result it was believed that the complex distribution might result from the unintuitive sodium atom motion caused by resonance fluorescence. In order to obtain results which matched observations they were required to use a longer sodium atom lifetime (due to photo-ionisation by ultra-violet radiation) than previously suggested from experiments ($1.69 \times 10^5$ s at 1 AU calculated by Huebner et al. [1993]). Combi et al. [1997] calculated a theoretical sodium ultra-violet photoionisation rate of $5.40 \times 10^{-6}$ s$^{-1}$ at 1AU, which equates to a lifetime of $1.85 \times 10^5$ s (slightly longer than that of Huebner et al. [1993]).

The Monte Carlo model of Brown et al. [1998] was produced to allow calculation of sodium velocity distributions resulting from different source models. It does not explicitly consider collisions within the coma in same way as the Combi et al. [1997] model. Instead the collision radius is considered as a hard spherical boundary, inside which the velocities are radially outwards at $0.8 \text{ km/s}$ (to account for collisional effects within the coma). Past the collision radius the neutral sodium atom velocities are affected by resonance fluorescence, experiencing a heliocentric velocity dependent acceleration.
reminiscent of that described by Combi et al. [1997] but using a slightly higher resolution velocity–acceleration spectrum (that is the version used by COMPASS, see chapter 5, figure 5.1). The model considers a fixed, constant heliocentric velocity nucleus (at constant heliocentric distance), with the collision radius determined by matching the model results to observations. Brown et al. [1998] do not consider acceleration due to resonance fluorescence within the collision radius. The contribution of sodium at each time step is weighted by:

\[ \exp\left(\frac{t}{\tau}\right), \quad (4.9) \]

where \( t \) is the time since liberation of the sodium atom and \( \tau \) is the lifetime of photoionisation. They use the lifetime of photoionisation as \( 1.69 \times 10^5 \) s, again from the theoretical value calculated by Huebner et al. [1993] as suggested by Combi et al. [1997].

The Brown et al. [1998] model considers three sodium source functions: a nuclear source, a dust source and a plasma source. The nuclear source is modelled as a point source with an initial random position (sodium atoms generated on a unit sphere, 1 km away from centre of the nucleus). The initial magnitude of the velocity is chosen as 0.8 km/s and the direction is chosen to be radially outwards, to be consistent with the choice of outward radial velocity inside the collision radius. The dust source is modelled using a \( 1/r^2 \) distribution. The initial velocity of the sodium atom is zero (unless the nucleus has a heliocentric velocity, in which case the velocity of the sodium atom is the heliocentric velocity of the nucleus). This only provides an approximation to a dust source as a true dust source is asymmetric.

The plasma source was considered differently by Brown et al. [1998]. It is estimated by considering the intensity and velocity of \( H_2O^+ \) measured on the date specified. In this case the model is one dimensional. The line of sight \( H_2O^+ \) intensity is used as the sodium source distribution and the \( H_2O^+ \) velocity is used as the starting sodium velocity. Although clearly sodium cannot be produced from \( H_2O^+ \), measurements of this species produce the clearest characterisation of the ion tail, which has been speculated to be a source of cometary sodium.

Brown et al. [1998] produce synthetic spectra as a result of their simulations, which allow extraction of the velocity of sodium at any point within the coma. It should be noted that Brown et al. [1998] consider the one dimensional nature of their plasma source and their collision radius approximation to mean that interpretation of their results cannot be performed close to the collision radius. These results allow them to interpret sources of sodium in Hale-Bopp from the velocities observed (see chapter 2 for a discussion of these results).

Kawakita and Fujii [1998] produced a Monte Carlo model of the brightness distribution of a sodium tail to allow them to interpret morphological changes in the sodium tail of comet Hale-Bopp. They considered a fixed nucleus (at a constant heliocentric distance)
and used a similar approach to Combi and Delsemme [1980] in order to consider the collisions between sodium atoms and water molecules. The collision radius is calculated considering a sodium-water cross section of $1 \times 10^{-14} \text{ cm}^2$, which is at the lower range of the Combi and Delsemme [1980] estimate. The collisions are considered to be elastically hard sphere collisions and the velocity of the water molecule is given by the vector sum of the radial outflow velocity and a randomised thermal component. Their simulation is performed between $t_{\text{obs}} - t_{\text{interval}}$ and $t_{\text{obs}}$, where $t_{\text{obs}}$ is the time of the observation being modelled and $t_{\text{interval}}$ is the simulation time interval. A sodium atom is released at a time, $t_i$:

$$t_i = t_{\text{obs}} - t_{\text{interval}} \zeta_i,$$

where $\zeta_i$ is a random number ($0 \leq \zeta_i \leq 1$), with an initial sodium velocity of 1 km/s in a randomised direction. The direction is determined by:

$$\cos(\theta_i) = 1 - 2\zeta_i,$$
$$\phi_i = 2\pi \zeta_i,$$

where $\theta_i/\phi_i$ are the spherical polar/azimuthal angles of sodium atom $i$ respectively.

In order to calculate the radiation pressure outside the collision zone (between the collision radius and the nucleus) they assume that the emission from transitions other than the sodium D doublet is negligible. Furthermore they use the high dispersion solar spectrum obtained by Kurucz et al. [1984] and obtain the oscillator strength of the sodium D doublet from Morton [1975]. The sodium equation of motion was integrated using a Runge-Kutta method and the number of particles initially in the simulation is 150,000 (although only 10,000 remain at $t_{\text{obs}}$ as most have been photo-ionised by ultra-violet radiation). Kawakita and Fujii [1998] use the theoretical photo-ionisation lifetime calculated by Combi et al. [1997] ($1.85 \times 10^5 \text{ s} \approx 2 \text{ days at 1 AU}$). Therefore $t_{\text{obs}}$ is chosen as 30 days in their simulations. Kawakita and Fujii [1998] were able to reproduce the changing brightness distribution of the narrow sodium tail using this approach, without the need for additional sources.

Schmidt et al. [2015] produced a 3D Monte-Carlo model for the neutral sodium tail they observed at comet ISON, which was based on that Schmidt [2013] had used to explain asymmetries in the neutral sodium tail of Mercury observed by the Messenger spacecraft, which was originally adapted from Schmidt et al. [2012].

In their simulation particle trajectories are calculated under the influence of solar gravity and radiation pressure, with one particle representing approximately $10^{22}$ neutral sodium atoms (although how this number is arrived at is unclear). Schmidt et al. [2015] use an adaptive step size fourth order Runge-Kutta integration method to calculate the particle trajectories at each timestep. Particles are released randomly in
time throughout the simulation. The total length of the simulation is chosen to be a few photoionisation lifetimes of sodium. The photoionisation lifetime of sodium used is identical to that adopted by Cremonese et al. [1997b], based on the theoretical calculations of Huebner et al. [1993]. The fractional content of each particle is reduced at each timestep to simulate the loss of neutral sodium atoms via photoionisation. The Swings and Greenstein effects are incorporated in the model via the dependence of the g-factor on the heliocentric distance and velocity of the particles. Optical depth effects in the coma are negligible for their observations (as the sodium emission is not greater in intensity than a few kR), so Schmidt et al. [2015] do not include them in their model.

Close to the nucleus, Schmidt et al. [2015] describe the distribution of sodium atoms analytically using the Haser [1957] model, where volume density, \( n \), at cometocentric distance, \( r \), is given by equation (4.2). Schmidt et al. [2015] use the Haser [1957] model under the assumption that close to the nucleus, the neutral sodium is collisionally coupled to the outgassing water vapour. Schmidt et al. [2015] use a mean gas outflow velocity, \( v_{\text{out}}(R) \), in km/s at heliocentric distance, \( R \), AU given by:

\[
v_{\text{out}}(R) = 0.85 R^{-0.5},
\]

which they state is consistent with the 1.1 km/s outflow velocity measured by Agúndez et al. [2014] at comet ISON at 0.61 AU. At larger spatial scales the outflow of neutral sodium is not collisionally coupled to the coma and the trajectory of particles is determined by the solar gravity and radiation pressure they experience. Schmidt et al. [2015] use a value of approximately 2500 km on 19.5 UT November 2013 and 12000 km on 20.5 UT November 2013 for the cometocentric distances at which collisions no longer dominate motion for the two dates they simulate, based on the smaller estimates for production rate and velocity given by Combi et al. [2014] and Budzien et al. [1994]. The initial velocities of the particles inside the collisional region are given by the radial velocity vector plus a randomly selected Maxwell-Boltzmann flux distribution at 125 K. Schmidt et al. [2015] note that temperatures lower than 125 K were recorded for comet ISON, but that their results are not significantly affected by a change in the outflow velocity.

Schmidt et al. [2015] note that an extended source of neutral sodium in the dust is likely from their observations, but state that a model of this type would be poorly constrained. Therefore, to included the effects of an extended source, Schmidt et al. [2015] add to the fractional abundance of the particles at each step, which effectively introduces a longer lifetime against photoionisation. The Schmidt et al. [2015] model is not an orbital model because it does not include particles being produced at different heliocentric distances (other than in the variation of the distribution with cometocentric distance), but does include variation of collision radius and g-factor based on the comet’s position at the times of the two observations simulated.
Chapter 5

Cometary Orbital Motion At Perihelion: An Adaptable Sodium Simulation (COMPASS)

5.1 Introduction

During the course of this PhD the author has developed a model, known as COMPASS: Cometary Orbital Motion At Perihelion: An Adaptable Sodium Simulation, in order to address fundamental discrepancies in the interpretation of sodium observations at comets, primarily in wide field imaging but also in spectra. To date no sodium tail model has fully included the variation in sodium production due to a comet’s changing orbital motion. Neither have they included the heliocentric velocity dependence of radiation pressure on the brightness of the tail or the evolution of sodium atoms in a fully three dimensional, heliocentric distance dependent manner. It is challenging to include all these effects in a way that can be applied to many different observations of sodium at comets taken at different times, but it is fundamentally important in order to be able to interpret observations successfully. The classical dust model (choosing a constant, large value of $\beta$ (e.g. 82, [Cremonese, 1999])) is not strictly appropriate for modelling neutral cometary sodium because the radiation pressure experienced by a sodium atom is dependent upon its heliocentric velocity in a non-intuitive manner. Therefore a more complex fully three dimensional, heliocentric velocity and acceleration dependent Monte Carlo model is required.

This chapter is presented in the same order as the steps taken within COMPASS to produce a result that may be compared with relevant observational data. First we discuss the setup of COMPASS: how orbital motion is included, how light travel time corrections are implemented and which source distributions are selected and why. Next we consider how the simulation is run, i.e. how atoms’ behaviour evolves within COMPASS.
based on their positions and velocities and how individual parameters (collision radius, outflow velocity, number of atoms per timestep) are varied with heliocentric distance.

Finally we consider how best COMPASS results may be interpreted, i.e. translation to relevant observational perspective, and the plots available for interpretation and convergence testing to produce robust results at different scales.

## 5.2 COMPASS Methodology

For most of the simulations considered in this thesis it is useful to consider the COMPASS simulations in two steps. In step one, termed the simulation step, representative sodium atom particles are produced in given spatial distributions along the comet’s orbital path for the duration of the simulation. This step is performed using the comet’s orbital plane as the frame of reference, and neglects observational perspective. The outputs from step one are saved as an IDL save file and basic diagnostic plots are produced to ensure the sodium atom particles are evolving correctly in the comet’s orbital plane. In step two, termed the plotting suite, the output from the simulation step is transformed to the observational perspective selected and a range of plots may be chosen to investigate the distribution of sodium emission seen by the observer. The outputs from step two may optionally be saved as an IDL file for further analysis, or the plot selected may be saved in a range of formats. The two steps in COMPASS are independent, which allows the result to be investigated from the perspective of multiple observers and/or a suitable variety of plots without the need to rerun simulations. However, the convergence level of results depends strongly on the observational perspective and the scale of the observation, therefore the same simulation (step 1) will not necessarily produce representative plots of neutral cometary sodium emission likely to be seen by different observers at different scales. The dust tail model discussed in chapter 9 introduces an additional step that is specific to that source distribution and is not discussed in this general chapter.

One key part of the methodology of COMPASS is that the neutral sodium emission in comets is simulated by looking at the overall intensity of the emission resulting from a series of representative sodium atom particles. These particles evolve in the same way as an individual neutral sodium atom (in step 1), but are representative of many neutral sodium atoms at that approximate position when neutral sodium D line emission intensity is considered (in step 2). The simplicity of this method greatly reduces the computational time required to complete these simulations, and therefore facilitates a good level of convergence of the desired outputs by making best use of the available computational resources.

In this chapter we discuss the broad principles used to develop the COMPASS simulation (step 1 described above) and plotting suite (step 2 described above) in chapters 5.2.2 and 5.2.3 respectively. We also consider the issue of convergence in COMPASS in
chapter 5.2.4 and how the level of convergence may be monitored to achieve a suitable level of convergence for a range of plots available in the plotting suite.

5.2.1 Steps taken prior to running COMPASS

Before the COMPASS simulation is run, the light travel time correction and total simulation time must be calculated to allow the correct orbital information to be extracted from the JPL Horizons database [Giorgini et al., 1996].

When comparing COMPASS simulation results with observational data, it is important to note that the time that the observation was taken represents the time at which the detected light reached the observer. As light travels at a finite speed, the position of the comet in the observation will therefore not be the same cometary orbital position at the time of the observation. If the emission is observed at time, $t$, seconds by an observer a distance, $D$, metres from the source it must have been emitted at time, $t_i$, seconds which satisfies the equation:

$$D = c(t - t_i)$$

where $c = 3 \times 10^8$ m/s is the speed of light. If the observer’s position is fixed at the time of the observation, the distance between that position and the comet, $D*$, may be calculated for a range of positions in the comet’s orbit. For each comet nucleus position considered for the correction (typically we consider a comet’s orbital position from $t_i = t - 15$ minutes to $t_i = t$, using a timestep of minutes), we calculate $D*$ and $D$. Then by minimising $D* - D$ it is possible to calculate the approximate time, $t_{i*}$, (to the nearest minute) before the observation at which the emission must have been released at the comet in order to have been detected by the observer at time, $t$. Using this approach, the end point of the simulation required for COMPASS to reproduce the observation is $t - t_{i*}$. It is not necessary to include light travel time correction if the comet is moving relatively slowly compared to the observer, but for completeness we include this correction throughout the projects presented in this thesis. It is possible to include the varying effects of light travel time on different parts of the tail using an iterative approach, but as sodium tails are not particularly extensive the effect is minimal and therefore was not included in COMPASS to reduce computational cost and simulation time.

Once the light travel time correction has been implemented, we calculate the total simulation time required to produce a representative neutral sodium atom simulation. The total simulation time was calculated based on the characteristic lifetime against photoionisation for a neutral sodium atom, $\tau$, produced at the heliocentric distance of the comet at the time of the observation. For COMPASS simulations, we use a characteristic lifetime against photoionisation at 1 AU, $\tau_{1AU}$, of $1.69 \times 10^5$ s, determined
from the theoretical calculations of Huebner et al. [1992], used by Combi et al. [1997] and [Brown et al., 1998]. The characteristic lifetime against photoionisation is scaled for other distances by:

$$\tau = \tau_{1AU} R^2,$$

(5.2)

where $R$ is the heliocentric distance of the sodium atom. This scaling is necessary due to the decrease in solar radiation away from the Sun as $1/R^2$. If $n$ neutral sodium atoms are present initially then $t$ seconds later the number of neutral sodium atoms not ionised on average will be:

$$n(t) = n \exp(-t/\tau).$$

(5.3)

The total length of the simulation was chosen such that approximately 0.1% of atoms produced at start of the simulation, at the heliocentric distance in the observation would be ionised by the final step in the simulation, therefore the total simulation time, $t_{tot}$, is given by:

$$t_{tot} = \tau_{1AU} R^2 (-\ln(0.001)) \approx 7 \tau_{1AU} R^2.$$ 

(5.4)

t_{tot} must be calculated individually for each comet during each observation time, and will change throughout the comet’s orbit. The values of $t_{tot}$ calculated using this approach become less valid for very small heliocentric distances, where the characteristic loss rates of neutral sodium are unknown and have steep gradients as a function of heliocentric distance.

### 5.2.2 The COMPASS Simulation

Once the steps detailed in chapter 5.2.1 have been completed, the COMPASS user has:

1. The time of the observation wished to be studied;
2. The light travel corrected time, $t - t^*_i$, at the comet that is equivalent to the time of the observation;
3. The total simulation time, $t_{tot}$, based on the heliocentric distance at $t - t^*_i$;

that are all required to complete a COMPASS simulation. COMPASS simulations require knowledge of the orbital motion of the comet during the simulation period, which is included in COMPASS through use of the JPL Horizons database [Giorgini et al., 1996] as it is more accurate than using averaged orbital elements. Therefore the next step is to use an interface to the JPL Horizons database (both the email and web interfaces are used for the simulations in this thesis) to extract the positions of
the comet and save that data as a text file that will later called by COMPASS to run the simulations. We wish to extract the position and velocity of the comet at the times of interest, using the ecliptic as our plane of reference with the Sun as the origin and therefore use the Horizons options listed in table 5.1. We find the positions and velocities of the comet at time \( t - t_i^* \) as geometric states and calculate the position of the observer and comet in identical reference frames. This means that the same routines may be used for the comet and observer datasets, which greatly reduces development and testing time required to ensure the simulation is accurate, as well as computational cost.

<table>
<thead>
<tr>
<th>Horizons Option</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ephemeris Type</td>
<td>Vectors</td>
</tr>
<tr>
<td>Coordinate Origin</td>
<td>Sun (body centre)</td>
</tr>
<tr>
<td>Output Units</td>
<td>km and km/s</td>
</tr>
<tr>
<td>Quantities Code</td>
<td>2 (state vector ( x,y,z,vx,vy,vz ))</td>
</tr>
<tr>
<td>Reference Plane</td>
<td>Ecliptic and mean equinox of reference epoch</td>
</tr>
<tr>
<td>Reference System</td>
<td>ICRF/J2000.0</td>
</tr>
<tr>
<td>Type</td>
<td>Geometric states (no aberration, instantaneous dynamical states)</td>
</tr>
</tbody>
</table>

Table 5.1: Table detailing the Horizons parameters used to extract comet nucleus positions and velocities for use with COMPASS. More information about the parameters is available in JPL Horizons [Giorgini et al., 1996].

The COMPASS simulation and plotting routines are written using the Interactive Data Language (IDL). The text files containing the Horizons data on the positions and velocities of a comet are read by the COMPASS routines and transformed into the comet’s orbital plane using two simple, geometric rotations in order based on the comet’s orbital elements. First, a comet at \((c_x, c_y, c_z)\) in the ecliptic frame is transformed to \((x, y, z)\):

\[
x = (c_x \cos \Omega) + (c_y \sin \Omega) \quad (5.5a)
\]

\[
y = (-c_x \sin \Omega) + (c_y \cos \Omega) \quad (5.5b)
\]

\[
z = c_z \quad , \quad (5.5c)
\]

where \(\Omega\) is the longitude of the ascending node, and then position \((x, y, z)\) is transformed to \((x', y', z')\) in the comet’s orbital plane using:

\[
x' = x \quad (5.6a)
\]

\[
y' = (y \cos i) + (z \sin i) \quad (5.6b)
\]

\[
z' = (-y \sin i) + (z \cos i) \quad , \quad (5.6c)
\]
where $i$ is the inclination of the comet’s orbit (see Appendix A for a discussion of a comet’s orbital elements). All evolution of neutral sodium in COMPASS is based in a coordinate system defined by the comets orbital plane, from a frame of reference with $(x', y', z') = (0, 0, 0)$ at the Sun’s position (i.e. with the same origin as the ecliptic plane). The reference frame is unique (but self consistent) for each comet being simulated. Rotation by the argument of perihelion, $\omega$, is therefore unnecessary and its omission saves computational expense.

The COMPASS simulations are based on a coordinate system defined by the comet’s orbital plane, as this is the most sensible coordinate system to consider when considering the evolution of cometary sodium in a orbital model. The comet’s motion will be confined within the comet’s orbital plane. It will therefore produce most of the cometary sodium within the orbital plane and as the position and velocity of cometary sodium is a result of solar radiation pressure and collisional effects in the densest part of the cometary coma, most of the evolution of cometary sodium will also be confined to directions parallel to the comet’s orbital plane. However, the exact radiation pressure force felt by a cometary sodium atom will depend on its heliocentric distance, and may be somewhat out of the comet’s orbital plane. Therefore in COMPASS each simulation step takes careful account of the positions of neutral sodium atom particles in the simulation.

Once the comet nucleus positions have been transformed to the comet’s orbital plane, the next step in COMPASS is to perform the situation using the randomised Monte-Carlo approach. Assuming there are 1, 2, 3...$n_t$ time steps within the simulation, with $N$ particles produced per time step:

1. Produce a random distribution of $N$ COMPASS particles at nucleus position 1.
2. Produce a random distribution of $N$ COMPASS particles at nucleus position 2 and evolve COMPASS particles produced at nucleus position 1.
3. Produce a random distribution of $N$ COMPASS particles at nucleus position 2 and evolve COMPASS particles produced at nucleus positions 2,1.
   :
   n. Produce a random distribution of $N$ COMPASS particles at nucleus position $n_t$ and evolve COMPASS particles produced at nucleus positions $(n_t - 1), (n_t - 2)...1$

At the end of the simulation, the final positions and velocities of the neutral sodium atoms are saved as an IDL save file that also includes information about the COMPASS simulation parameters used to facilitate transformation into a different frame to allow simulated images, spectra and other useful diagnostic information to be extracted by the COMPASS plotting routines.
The COMPASS particles are produced at the current comet nucleus position using one of two main source distributions. A third source distribution was developed to simulate neutral sodium emission from the cometary dust tail and its methodology is described in detail in chapter 8.

The first source distribution is designed to simulate direct release of neutral cometary sodium and is described throughout this thesis as the ‘sodium from nucleus’ source or source 1. The distribution of this source originally had particles produced in a confined sphere around the current comet nucleus position. The method produced a distinct error (discussed in more detail in the evolution explanations that follow) due to the use of the collision radius, so the ‘sodium from nucleus’ source was updated to a normal distribution with a full width half maximum of $8 \times 10^4$ km (chosen at it is twice the width of the collision radius calculated by Brown et al. [1998]) that allowed much more realistic results to be produced with the collision radius approximation on a scale suitable for the simulations presented in this thesis.

The second source distribution considered in this thesis is known as ‘sodium from dust’ or source 2, and was designed to simulate emission of neutral sodium originating in the extended outflow of cometary dust and neutrals from the cometary nucleus, i.e. that the sodium distribution is considered as if it were collisionally coupled to the outgassing volatiles. Using the same approach as the Brown et al. [1998] model, the second source is a simple $1/r^2$ distribution, where $r$ is the cometocentric distance. This source is reminiscent of a simplified Haser [1957] model, that describes volume density with cometocentric distance, $\rho(r)$, as [Schmidt et al., 2015]:

$$\rho(r) = \frac{Q}{4\pi v_{out}} \exp \left(-\frac{r}{v_{out}\tau_i}\right),$$

where $Q$ is production rate, $\tau_i$ is photolysis lifetime (by which we mean the characteristic lifetime against separation of sodium bearing molecules by light) and $v_{out}$ is the mean gas outflow velocity. Photodissociation is the dominant form of destruction of molecules in the coma. The Haser [1957] model has been very successful at describing the intensity distribution close to cometary nuclei, and is typically used to describe the outflow of cometary dust and neutrals. The dominant term in the volume density variation with cometocentric distance is the $1/r^2$ factor, therefore for simplicity and as the dominant processes that release neutral sodium from cometary material are unknown we only consider the $1/r^2$ dependence on the sodium distribution. The $1/r^2$ distribution used in COMPASS extends to a maximum of $1 \times 10^7$ km, which was chosen based on the scales of the observations to be simulated. Further exponential terms may be added to include the depletion of sodium with cometocentric distance, but that is beyond the scope of this work.

Sources 1 and 2 were also chosen to facilitate direct comparison with the results of the Brown et al. [1998] model, which was very successful at reproducing the emission of
neutral sodium observed at comet Hale-Bopp, although their model did not consider the sometimes crucial effects of orbital motion (see chapter 4 for more details).

For sources 1 and 2 the initial cometocentric velocity of the neutral sodium atom particles produced in COMPASS was zero. There are several reasons for this. Wurz et al. [2015] have observed high velocity neutral cometary sodium which they speculate is the result of sputtering of the nucleus of comet 67P by solar wind, but they also identify an anti-correlation between regions of high cometary activity and high velocity neutral sodium observations, suggesting that once a significant amount of cometary activity has been established (which is the case for all comets studied in this thesis) sputtering may no longer be a dominant source of cometary sodium, possibly because the solar wind no longer has direct access to the nucleus surface once a comet is active. The Brown et al. [1998] model also indicated that high velocity neutral sodium, such as that released from the cometary ion tail, was very unlikely to be the source of neutral cometary sodium at comet Hale-Bopp. Furthermore, neutral cometary sodium is rapidly accelerated by solar radiation pressure and therefore any small initial variations in velocity distribution are unlikely to be detectable down the tail and to date no high velocity neutral cometary sodium has been detected in the vicinity an active cometary nucleus (Brown et al. [1998] measured a maximum velocity of approximately 3 km/s at $1 \times 10^5$ km from the nucleus).

Once the source distributions are established, the positions of neutral sodium atom particles produced at previous steps are evolved as previously discussed. By this we mean that the particles’ position and velocity are updated based on their current position to incorporate the physics of the formation of a neutral sodium tail. Sodium atoms are evolved differently in COMPASS depending upon their cometocentric distance, $r$. There are two different evolution schemes: inside the collision radius ($0 \geq r < r_c$) and outside the collision radius ($r \geq r_c$).

Outside the collision radius the atoms are influenced by the effects of solar radiation pressure. This is incorporated in COMPASS using a heliocentric distance and velocity dependent, anti-sunward acceleration term, from which the new velocity and position of the sodium atom are calculated. Acceleration in the antisunward direction in this region, $a_x(v)$ in ms$^{-2}$, as a function of heliocentric velocity, $v$ in m/s, is given by:

$$a_x(v) = \frac{-3 \times 10^{-4} \times spec(v)}{R^2}, \quad (5.8)$$

where $R$ is the heliocentric distance in AU and $spec(v)$ is the heliocentric velocity dependent acceleration function. The heliocentric velocity dependent acceleration function used in this model was provided by Brown et al. [1998], which is of slightly higher resolution than that introduced by Combi et al. [1997] but is of the same form (see figure 4.2 in chapter 4). It is shown in figure 5.1 and was produced using the method described in chapter 2.2. The multiplicative factor of $3 \times 10^{-4}$ is chosen to accurately
give a minimum acceleration of $3 \text{cm/s}^2$ at 1 AU, based on the results of Combi et al. [1997]. Acceleration in the anti-sunward direction varies as $1/R^2$ due to decrease in photon flux with increasing heliocentric distance.

Inside the collision radius the sodium atoms are not influenced by the effects of solar radiation pressure, and instead are entrained in the radial outward flow within the collisional region of the coma. The mean gas outflow velocity, $v_{\text{out}}$, within this region is also a heliocentric distance dependent parameter. The velocity in the comet’s orbital plane, $\vec{v}$, of a sodium atom within this region is therefore given by:

$$\vec{v} = \left[ \frac{\vec{x}_{\text{comet}}}{r} \times v_{\text{out}} \right] + \vec{v}_{\text{nuc}},$$

(5.9)

where $\vec{x}_{\text{comet}}$ is the sodium atom position vector with respect to the cometary nucleus and $\vec{v}_{\text{nuc}}$ is the current velocity of the cometary nucleus, based on a consideration of the projection of the outflow velocity onto each axis in the simulation using three dimensional trigonometry. All velocities are in km/s and all distances are in km.

The outflow velocity, $v_{\text{out}}$, within the collision radius varies with heliocentric distance in COMPASS as:
\[
v_{\text{out}} = \frac{0.8 \text{ km/s}}{R_{0.5}} ,
\] (5.10)

which was originally used by Combi [2002]. Combi [2002] warns that extending this simple scaling may be inappropriate in some cases, but as it remains the best currently available scaling system for variation of outflow velocity with heliocentric distance it is implemented in COMPASS.

The collision radius in the COMPASS simulation is calculated using different methods depending on the activity and heliocentric distance of the comet to be simulated. Over the range of the simulation it may be appropriate to consider a constant collision radius, such as the value of \(4 \times 10^4\) km used by Brown et al. [1998], but it may also be useful to consider a variation in the collision radius over the short range in heliocentric distances in the simulation. It is also important to be able to extend our current understanding of the collision radii of comets far from the Sun to understand the observations of near-Sun comets we wish to investigate.

COMPASS includes two different options for scaling the collision radius, \(r_c\), to different heliocentric distances. A constant collision radius is appropriate if the change in heliocentric distance is small over the simulation, and this is often the case in practice.

The first option for scaling the collision radius is to calculate the change in the collision radius based on the simple scaling arguments given in Whipple and Huebner [1976]. If the collision radius is assumed to be equal to the mean free path for collisions in the coma then:

\[
r_c = \frac{1}{n(r_c)\sigma_{\text{coll}}} = \frac{4\pi \nu r_c^2}{Q\sigma_{\text{coll}}} ,
\] (5.11)

where \(n(r_c)\) is the number density of all species in the coma, which is a function of the cometocentric distance, \(\sigma_{\text{coll}}\) is the collisional cross section and \(Q\) is the production rate of all species in the coma. \(n(r_c)\) and \(Q\) may be approximated to the production rate and number density of the dominant species in coma (i.e. water) respectively to make calculation practical. This equation rearranges to:

\[
r_c = \frac{Q\sigma_{\text{coll}}}{4\pi v_{\text{out}}} ,
\] (5.12)

but \(Q\) and \(v_{\text{out}}\) have a heliocentric distance dependence that must be incorporated. From equation (5.10) we have the variation of outflow velocity with heliocentric distance, but to calculate the variation of production rate with heliocentric distance is more complex. From Swamy [2010], we estimate to a first order the variation in pro-
duction rate with heliocentric distance in a simplistic method using two regimes:

\[
R \leq 1 \text{ AU} : Q \propto R^{-4} \tag{5.13a}
\]
\[
R > 1 \text{ AU} : Q \propto R^{-2} \tag{5.13b}
\]

and substituting these dependences into equation (5.12) gives two collision radius schemes:

\[
R \leq 1 \text{ AU} : R_C \propto R^{-3.5} \tag{5.14a}
\]
\[
R > 1 \text{ AU} : R_C \propto R^{-1.5} \tag{5.14b}
\]

However, when this is applied to comets with very small heliocentric distances, such as those seen by the LASCO coronagraph, based on a value of $4 \times 10^4$ km at 1 AU, the collision radius rapidly increases in size until it encompasses the comet’s heliocentric distance. This approach is therefore clearly flawed for near-Sun comets, so for these comets a different approach must be used.

For near-Sun comets, roughly defined for our purposes as having a heliocentric distance inside the perihelion of Mercury’s orbit (0.307 AU), we use an estimate of the collision radius based on the approximate width of the neutral sodium tail of comet McNaught in the LASCO orange filter image shown in figure 9.2, chapter 9. The width of the neutral sodium tail of comet McNaught in this image was measured by Jones [2015] to be approximately $1 \times 10^5$ km at a heliocentric distance of 0.1898 AU, therefore for a heliocentric distance less than or equal to this distance we estimate the collision radius to be $0.5 \times 10^5$ km, which is half of the width of the neutral sodium tail. The collision radius is estimated to be approximately half the width of the neutral sodium tail for near-Sun comets is appropriate because of the dynamics of the collision radius, as illustrated in the diagram in figure 5.2. If a neutral sodium atom is produced on the sunward side of the nucleus, it will be trapped with the outflow of cometary material until it reaches the edge of the collisional region. At this point it will start to be influenced by the effects of solar radiation pressure, which will force it back inside the collisional region and cause it to be pushed outward by the outflow of cometary material. This process will repeat and eventually cause the sodium atom to effectively ‘slip around’ the collisional region and form part of the tail. The collisional region does not have a sharp boundary in comets, therefore this estimate of the collision radius produces an upper limit but is sufficient for our requirements.
The collision radius effectively quantifies the effects of a collisional cometary coma in a simple, computationally inexpensive manner, but is not without drawbacks. Firstly, the collisional region in a comet is not spherical, as the coma of the comet is effectively compressed by incident solar photons and particles, so a collision radius parametrisation can only be used as an approximation. Secondly, inclusion of a collision radius in an orbital model effectively rules out the use of simple sources based in a narrowly defined region very close to the cometary nucleus for certain simulation scenarios. For example, if a COMPASS simulation contains consecutive comet nucleus positions that are sufficiently close to each other that the narrow distribution of particles produced at the first timestep is evolved to lie solely within the collision radius at the second timestep, the resulting neutral sodium tail produced will be of the form of a straight line which travels outwards to the edge of the collision region followed by a curved line at a different angle due to radiation pressure. As shown in figure 5.3, this will produce an effective offset to the neutral sodium tail that is unphysical and makes a source distribution of this type unsuitable for an orbital model. The same effect is present in all other distributions for simulations of this type, but using slightly broader distributions reduces its prominence and its ability to negatively influence the results.

5.2.3 The COMPASS Plotting Suite

At the end of the COMPASS simulation the positions and velocities of all the neutral sodium atom particles are saved to be recalled by the COMPASS plotting suite, which contains a series of IDL routines written to allow interpretation of this raw data into what is likely to be seen by remote or in-situ observers. Using this approach allows for many different diagnostic plots to be generated from one simulation result, which greatly reduces the computational cost of COMPASS whilst increasing its ability to interpret results successfully.

The COMPASS simulations are performed in the comet’s orbital plane, so the first step of the COMPASS plotting suite is to perform the rotation in equations (5.6) with $i = -i$ followed by the rotation in equations (5.5) with $\Omega = -\Omega$ to allow the position of particles simulated using COMPASS to be transformed back to the ecliptic plane frame, which is very useful for transforming to the observational perspective of different observer’s locations.
Figure 5.3: Plot of COMPASS particles in the comet’s orbital plane, with the units of each axis shown in km and the x axis directed radially away from the Sun. The nucleus positions in the simulation are indicated by crosses, with the red cross at the centre of the circle indicating the current comet nucleus position, surrounded by the black circle indicating the collision radius. The colour of the sodium atom particles in the plot (shown as diamonds) is identical to the colour of the comet nucleus position at which it was produced. This plot shows why a narrowly distributed source centred at the comet nucleus is unsuitable for use with a large number of time steps over a short range in an orbital, collision radius based model like COMPASS.

Text files generated by JPL Horizons [Giorgini et al., 1996] and/or the IDL SPICE Kernels (implemented using Solarsoft [Freeland and Handy, 1998]) contain position and velocity data information on the observer (spacecraft/planet) at the date of the observation. They are produced with the same units and equivalent parameters as those given in table 5.1 and therefore are easily compared with the results of COMPASS that have been transformed back into the ecliptic.

The COMPASS plots available in the plotting suite that are used in this thesis are broadly grouped into 2 categories: diagnostic plots and observer plots.

Diagnostic plots are plots that help the user to understand whether the results produced by COMPASS are reliable, and are particularly useful for debugging and understanding perspective issues. These plots exist in three groups:

- Comet Orbital Plane
- Ecliptic Frame
• Sun–comet Line

Comet Orbital Frame plots show a projection of the three dimensional positions of the COMPASS particles in the comet orbital plane, whereas Ecliptic Frame plots show the positions of COMPASS particles in the same frame of reference as that used in the JPL Horizons [Giorgini et al., 1996] outputs and Sun–comet line plots show the positions of COMPASS particles collapsed into the comet’s orbital plane and rotated so that the x axis points in the anti-sunward direction (as shown in figure 5.3). The colours of COMPASS particles shown in these plots may be set to indicate the nucleus position from which they originate (used to indicate whether sufficient mixing has occurred between particles produced at subsequent comet nucleus positions such that convergence is meaningful) or may indicate the velocity of the particles or their age since production (used to check that COMPASS evolution is producing acceleration in the range expected). For the comet orbital plane plots there is also the option to draw a series of boxes in a given region to investigate the distribution of particles produced by the simulation. No brightness effects are included in diagnostic plots because there is no way to measure effects observed by diagnostic plots and therefore the results would be meaningless.

Observer plots exist in two groups:

• Sky Plane Plots

• Instrument Plane Plots

These plots are representative of what would be seen by an observer, and have coordinates equivalent to celestial right ascension and declination as would be seen by an observer at a given location. Sky plane plots show full spherical sky views (including positions of bright stars) of the expected position of the neutral sodium particles produced by COMPASS, and are useful for determining whether the perspective effects are included correctly based on a comparison of expected comet nuclei and star positions and known values. Instrument plane plots are identical to sky plane plots but the field of view of these plots is limited to the field of view of the instrument being studied for the observation. Currently CoCam, LASCO C2 and LASCO C3 fields of view are available, in addition to specialised fields of view which focus on the comets observed by each of these instruments (for example a comet Hale-Bopp focussed CoCam field of view and comet McNaught, NEAT and Hyakutake focused LASCO C3 fields of view are available). The same position plots are available for all observer plots as are available with the diagnostic plots, but for instrument plane plots other useful features are also available. The two key plots that form the core of the results of this thesis are the ‘binned’ plots, which sum the intensity weighting along a line of sight from the observer to produce a map of the intensity in different regions seen as an image from the perspective of the observer, and the ‘multi slit’ plots, which simulate spectrographic results by drawing an artificial slit on the sky based on the observer’s perspective and
splitting the artificial slit into a number of divisions along its longest axis to simulate the intensity distribution along a slit that could be extracted from spectra of neutral cometary sodium features. Care was taken to ensure that each of the regions considered in the ‘binned’ and ‘multi slit’ plots were of the same surface area on the observer’s sphere, so that meaningful comparisons could be made between different chapters when considering the number (and intensities) of particles in each region.

Both the ‘binned’ and ‘multi slit’ plots include a number of intensity weightings applied to each of the COMPASS particles that contribute to the brightness of a given region in the plot. These intensity weightings are calculated for each of the COMPASS particles, multiplied together to get an overall weighting and then summed in a selected region along the line of sight of the observer to produce simulated images and spectra. There are currently four different intensity weightings incorporated in COMPASS:

1. $1/D^2$ (Dist2): Decrease of emitted photons detected with increasing distance, $D$, between the neutral cometary sodium atom and the observer.

2. $e^{-t/\tau}$ (Fraction): Loss of neutral sodium atoms at the comet (leading to loss of emission from a given particle, as one particle represents multiple atoms), where $t$ is the time since the atom was produced and $\tau$ is the characteristic lifetime against photoionisation ($\tau$ in seconds varies with heliocentric distance, $r$, as $\tau = 169000r^2$, based on the values used by Brown et al. [1998]).

3. $1/R^2$ (Obs): Scaling in the flux of solar photons reaching the as a function of heliocentric distance, $R$.

4. $spe(v)$ (Spec, see equation (5.8)): Amount of emission from sodium atom depends on the fraction of incident solar radiation the atom absorbs, which for the case of neutral cometary sodium is a function of its heliocentric velocity due to the Swings and Greenstein effects (see chapter 2.2 for more details).

Once the total intensity weightings have been summed along the line of sight from the perspective of the observer over the desired regions in the ‘binned’ or ‘multi slit’ plots the relative intensity of each of the regions is calculated as a percentage of the maximum intensity, which is typically at the final comet nucleus position in the simulation. It is hoped that a properly calibrated measurement of cometary sodium will facilitate calculation of the factor required to transform the relative intensity into an absolute intensity for a given comet, or type of comets.

### 5.2.4 Convergence

Traditionally in computational modelling, physical parameters will be selected for a model and then any other variables will be cycled through until they converge upon a result. For example the timestep in the simulation may be decreased until the result of the simulation no longer changes significantly, and at this point the simulation would
be said to have converged upon a solution. In COMPASS we select the collision radius and source distribution function as the physical parameters of the problem, and then converge the timestep and number of atoms produced per timestep separately. When the simulations have converged, adding more atoms per timestep or decreasing the timestep should be identical, and therefore converging the timestep and number of atoms per timestep separately provides the most unbiased computational solution.

COMPASS simulations are run in a coordinate system based on the orbital plane of the comet, as physically this is where most of the evolution takes place, but the results may only be compared with observational data once they have been transformed into the relevant sky plane (with the origin either near L1 for the LASCO simulations, or at Earth for the ground based observations). Therefore it is the transformed simulation result (i.e. the output from the plotting suite), not the initial output in the comets orbital plane that must be converged for the simulation results to be robust and have physical significance.

As COMPASS is designed to allow comparison between different types of data on different scales, different convergence criteria may be used to produce useful results whilst making the best use of the available computational resources.

It is important that convergence is achieved for each separate simulation result by first converging the length of the timestep in the simulation (using a sufficiently large number of particles produced per timestep), and then to converge the number of particles produced per timestep (by using the previously calculated converged timestep). As we use multiple sources in COMPASS we choose to converge the broadest source (the $1/r^2$ approximate dust source) to make the best use of the available computational resources, as if this source is converged all other sources must also.

Timestep convergence in COMPASS is identified by comparing the result of the current output (by which we mean the COMPASS plot in the relevant frame of reference with the chosen plot parameters, not in the initial output of particle positions in the comet’s orbital plane where the simulation takes place), with the previous output produced by the simulation that was run using half the number of timestep intervals. In a similar manner, convergence in the number of particles produced per timestep was achieved by comparing the result of the current output with the result of the previous output that used half the number of particles produced per timestep. In both types of convergence testing the following criteria were selected based on an appropriate convergence threshold, T%. The simulation was said to have converged when the following criterion is satisfied:

\[
\text{rms}(\Delta I) = \sqrt{\frac{1}{n}(\Delta I_1^2 + \Delta I_2^2 + \ldots + \Delta I_n^2)} \leq T \tag{5.15a}
\]

\[
\Delta I = I_k - I_{k-1} \quad , \tag{5.15b}
\]
where \( \text{rms}(\Delta I) \) is the root mean square of \( \Delta I \), which is composed of \( n \) values of difference in intensity, \( I \), at identical regions in the COMPASS output in simulation \( k \) and simulation \( k-1 \).

The COMPASS simulation and plot suites were written in IDL8.3, and composed of 113 and 215 routines respectively (of which 32 routines are shared between the two suites). The software was developed locally using the IDL development environment in conjunction with the solarsoft packages written by Freeland and Handy [1998] (ss-widlde). It was then uploaded to MSSLT2 (based at MSSL/UCL) and run remotely via bash scripts. MSSLT2 has \( \times86\_64 \) architecture with 64 CPUs operating at 1400MHz. Figures 5.4 and 5.5 show that the COMPASS simulation software is relatively quick to run in this manner, but the COMPASS plotting software is considerably slower which limited the choice of convergence threshold. In the configuration used IDL is also unable to create more than \( 3 \times 10^7 \) particles as it cannot allocate sufficient memory. For the simulations presented in this thesis a convergence threshold of 10% was often chosen as a compromise between computational resource allocation and result quality, which required sufficiently high image/profile resolution.

![Figure 5.4: Plot showing typical times for COMPASS simulations to complete. The variation seen is the result of using the computer at peak/off-peak times, and using different parameters within COMPASS.](image)
5.3 Summary

In this chapter we have described the development of the COMPASS model of neutral cometary sodium and how it may be implemented to achieve a level of convergence indicative of a physically representative result. COMPASS is the first neutral sodium tail Monte-Carlo model to successfully incorporate full heliocentric distance and velocity dependence as well as the effects of the orbital motion of the comet. The simplicity and adaptability of this model makes it powerful, but it may be necessary to revisit the assumptions made in this chapter when further developing COMPASS in order to more accurately represent neutral sodium emission at different comets.

For the remainder of the work presented in thesis we apply the COMPASS model to a variety of different scenarios of neutral sodium tail observations at comets. COMPASS is easily adapted to new comets, observations and initial source distributions, which means that it is well suited to adapting to new ideas about the sources of sodium as more information becomes available.
Chapter 6

Application of COMPASS to Spectroscopic Observations of Comet Hale-Bopp (C/1995 O1)

6.1 Introduction

In this chapter we discuss the application of COMPASS (see chapter 5) to spectroscopic observations of comet C/1995 O1 Hale-Bopp (henceforth Hale-Bopp). The sodium emission from this comet was studied extensively by multiple authors using spectroscopy, following the initial detection image produced by Cremonese et al. [1997b]. These observations provide the data to further test COMPASS by allowing investigation of the morphology of the neutral sodium emission at comet Hale-Bopp at different cometocentric distances and dates. The aim of this study is to reproduce spectroscopic observations of comet Hale-Bopp drawn from literature using COMPASS in a self-consistent manner that will allow conclusions to be drawn about the source(s) of sodium at comet Hale-Bopp, and whether they are variable. This study aims to investigate the neutral sodium emission from comet Hale-Bopp at different scales.

6.2 Aims of this study

In order to draw together the observations of comet Hale-Bopp in a comprehensive manner that can be most easily simulated using COMPASS and allows conclusions to be drawn about the overall behaviour at comet Hale-Bopp, we seek to simulate the sodium measurements taken by Brown et al. [1998] and Rauer et al. [1998]. For more details on the Lick Observatory 0.6 m Coudé auxiliary telescope coupled to the Hamilton Echelle Spectrometer used by Brown et al. [1998] and the Observatoire de Haute-Provence CARELEC spectrograph at the 1.93 m telescope and ISIS double beam
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spectrograph at the 4.2 m William-Herschel Telescope used by Rauer et al. [1998] see chapter 3.

The Brown et al. [1998] intensity profile taken from the spectra observed using the Lick Observatory 0.6 m Coudé auxiliary telescope coupled to the Hamilton Echelle Spectrometer on 8 April 1997 was selected for comparison with COMPASS for two reasons. Firstly, Brown et al. [1998] produced the first successful Monte-Carlo model of neutral cometary sodium. COMPASS was based on this model and therefore comparison with this result allows the importance of orbital motion and observational perspective to be determined for this observation, as consideration of orbital motion and observational perspective were comprehensively included in COMPASS but largely absent from the Brown et al. [1998] model. Secondly, the brightness profile obtained by Brown et al. [1998] was used to evaluate the effectiveness of COMPASS along the Sun–comet line close to the cometary nucleus, over a relatively small area of the sky (i.e. the area of the slit).

The Rauer et al. [1998] intensity profiles taken from spectra obtained using the CAR-ELEC spectrograph on the 1.93 m telescope at the Observatoire de Haute-Provence on 14 March 1997 and using the ISIS double beam spectrograph at the 4.2 m William-Herschel-Telescope of the Isaac Newton Group on 16 April 1997 were selected for comparison with COMPASS because, as with the Brown et al. [1998] intensity profiles, they allow characterisation of the effectiveness of COMPASS close to the cometary nucleus over a very small area of sky. However, the intensity profiles taken by Rauer et al. [1998] allow additional insight than that of Brown et al. [1998] because the three profiles presented by Rauer et al. [1998] are taken on two different dates and one is taken perpendicular to the Sun–comet line. Therefore the Rauer et al. [1998] intensity profiles allow an understanding of the variability of the neutral sodium intensity profiles of comet Hale-Bopp and insight into the distribution of sodium emission both along the Sun–comet line and perpendicular to it.

6.3 Observations

Once the distinct neutral sodium tail had been clearly identified by Cremonese et al. [1997b], it was also studied by other authors spectroscopically. The neutral sodium emission intensity profiles (and velocity profile for the Brown et al. [1998] measurement) resulting from their observations are reproduced in figures 6.1, 6.2, 6.3 and 6.4. During the period considered in this study, comet Hale-Bopp could only be observed close to twilight due to the nature of its orbit, which introduces some additional error into the calibration of these measurements. The instruments which produced these measurements are discussed in chapter 3.

The Brown et al. [1998] study (result reproduced in figure 6.1) looked at the relative
intensities of neutral sodium and continuum dust emission along the projection of the Sun–comet vector. Calibration of the results was a multi-step process. They isolated the relevant order of the Echelle spectrum by using a 40 Å wide filter centered at 5893 Å, which is the approximate centre of the D1 and D2 neutral sodium emission lines (at 5896 Å and 5890 Å respectively), and recorded the result on a 2400x2400 TI CCD. Brown et al. [1998] then subtracted light contributions from the faint twilight sky by determining the twilight sky level at the time of the observations by taking spectra far from the region of cometary emission and scaling a sky spectrum taken in daylight. The contribution due to solar continuum reflected by cometary dust was estimated by calculating the product of the average spatial profile away from the cometary/sky sodium lines and sky spectrum corrected for Doppler shift introduced by the relative velocity between the comet and the Earth. This contribution was also subtracted from the spectra during calibration. Two Gaussians were then fitted to the calibrated spectra at the position of the cometary sodium emissions and the sodium emission from the bright San Jose sky. The geocentric velocity of sodium at the comet was then calculated by estimating the separation of the Gaussian centres (the uncertainty in this procedure is estimated to be approximately ±0.25 km/s for regions of good signal to noise ratio), and knowledge of the geocentric velocity of the cometary nucleus then allowed the absolute velocity of the cometary sodium to be calculated with respect to the velocity of the cometary nucleus. The relative intensity of the cometary sodium emission was also calculated by summing the counts at each spatial location and dividing this result by the slit function, which was determined by sky measurements using an identical setup.

Brown et al. [1998] state their observations achieved a spectral resolution FWHM of 5×10^4 at a spatial scale of 2.16 arcsec/pixel, velocity resolution of 6.2 km/s and a spatial scale of 2200 km/pixel projected at the comet during the time these observations were taken. They show the intensity and velocity profiles of neutral sodium emission on 8.15 April 1997 along the Sun–comet line. This result is reproduced in figure 6.1. A clear sunward spike is identified in this intensity profile, which Brown et al. [1998] also say is observed in other spectra taken at similar times and can therefore not be described as a transient feature. The sunward spike may be understood as a sunward stagnation region, which is primarily the result of the Swings/Greenstein effect on cometary sodium. The theoretical formation of a stagnation region is discussed in chapter 2.2.

The Brown et al. [1998] observation formed the basis for the original Monte-Carlo neutral sodium tail model, which in turn formed the starting point of COMPASS. The Brown et al. [1998] model is discussed in more detail in chapter 4.

The three neutral sodium emission intensity profiles presented in the Rauer et al. [1998] study are shown in figures 6.2, 6.3 and 6.4. All spectra were bias subtracted, flatfielded and wavelength calibrated. Rauer et al. [1998] identify the variable water content of
Figure 6.1: The intensity (top panel) and velocity (bottom panel) profiles of neutral sodium and dust emissions along the Sun–comet line observed at comet Hale-Bopp by Brown et al. [1998] on 8.15 April 1997. The intensity of cometary sodium is indicated by the solid line in the top panel, whereas the estimated intensity of cometary dust is shown as a dotted line. This observation is referred to in this chapter as observation 1.

the atmosphere as being a significant difficulty in the calibration of their data. Water emission from Earth is typically an issue for observations in the range 5.5–7.5 µm, as the emission is centered 6.3 µm but broadens significantly by collisions in the atmosphere [Bachmeier, 2016]. Neutral sodium D1 and D2 emissions occur at 5896 Å and 5890 Å respectively so telluric water emission may be an issue for this species, but as varying telluric emission has different effects on D1 and D2, Rauer et al. [1998] only consider features which are observed in both spectral lines to be a direct result of a variation in cometary sodium distribution.

The observation presented in figure 6.2 was produced by the CARALEC spectrograph at the Observatoire de Haute-Provence (France) on 14 March 1997. Rauer et al. [1998] used a 5.5 arcmin slit, with a resolution of 1.1 arcsec/pixel and a dispersion 1.8 Å/pixel. The solar continuum reflected dust contribution to the observed emission was estimated for this measurement by taking the solar spectrum from a solar atlas [Kurucz et al., 1984] and convolving it with a Gaussian profile so it had the same resolution as the spectra measured.

The observations presented in figures 6.3 and 6.4 produced by ISIS Double Beam Spectrograph at the William-Herschel Telescope (La Palma, Spain) on 16 April 1997. Rauer et al. [1998] used a 4 arcmin slit, with a resolution of 0.36 arcsec/pixel and a dispersion 0.4 Å/pixel. The solar continuum reflected dust contribution to the observed emission was estimated for this measurement by measuring the reflected light from the Moon. The intensity profile along the Sun–comet line in figure 6.3, observed on 14 March 1997, is very different from that in figure 6.2, observed on 16 April 1997. Both show
Figure 6.2: Neutral cometary sodium emission intensity profile along the Sun–comet line, observed using the CARALEC spectrograph on 14 March 1997, reproduced from Rauer et al. [1998]. The solid line indicates the neutral sodium emission and the dashed line indicate the continuum dust emission. This observation is referred to in this chapter as observation 2.

Figure 6.3: Neutral cometary sodium emission intensity profile along the Sun–comet line, observed using the ISIS double beam spectrograph on 16 March 1997, reproduced from Rauer et al. [1998]. The solid line indicates the neutral sodium emission and the dashed line indicate the continuum dust emission. This observation is referred to in this chapter as observation 3.

6.4 Preparation of the Observations

In order to compare the intensity profiles observed by Brown et al. [1998] and Rauer et al. [1998] the relevant data were extracted from plots produced by the authors using the online Web Plot Digitiser [Rohatgi, 2015], which is available under a GNU General Public License. The software allows an image to be uploaded and, through user input of
Figure 6.4: Neutral cometary sodium emission intensity profile perpendicular to the Sun–comet line, observed using the ISIS double beam spectrograph on 16 March 1997. Reproduced from Rauer et al. [1998]. The solid line indicates the neutral sodium emission and the dashed line indicate the continuum dust emission. This observation is referred to in this chapter as observation 4.

the scales present within the plot image, draws an appropriate grid and calculates the points within the line plot based on the user’s input of the foreground and background colours within the plot. The lines within the plot may then be detected manually and false points may then be edited or removed. The errors resulting from this method are negligible compared to calibration errors.

6.5 COMPASS Implementation

The general procedures for the implementation of COMPASS are discussed in chapter 5. In this chapter we discuss the application of those general procedures to produce COMPASS simulations of the observations of comet Hale-Bopp outlined in chapter 6.3 and discussed in detail in chapter 3.

6.5.1 COMPASS Simulation Parameters

The primary variable required for COMPASS simulations is the collision radius, $r_c$, as other simulation variables (timestep, number of particles per timestep) are selected based on which values produce converged solutions and not based on their physical significance. For comet Hale-Bopp we choose a constant value of $r_c = 4 \times 10^4$ km based on the successful comparison of the Brown et al. [1998] simulations with observational data at 1 AU, because comet Hale-Bopp remained at approximately 1 AU throughout the observations discussed in this chapter. For the same comet, observed during the
same perihelion passage at approximately the same perihelion distance, the collision radius should not change significantly unless a dramatic change in activity occurs, such as that produced during an outburst.

We also corrected the date of the observation to be simulated due to light travel time to the nearest minute (see chapter 5 for more details) and then used the light travel time corrected observation date and the total time of the simulation calculated using equation (5.4), to run the appropriate dates through the JPL Horizons online database [Giorgini et al., 1996] and extracted the three dimensional positions \((x, y, z, v_x, v_y, v_z)\) of comet Hale-Bopp and Earth (as the origin of the observations). The orbital parameters of comet Hale-Bopp were also extracted from the JPL Horizons small body browser [Giorgini et al., 1996], in order to convert the three dimensional positions produced by the JPL Horizons database into the comet’s orbital plane, where simulation of neutral cometary sodium evolution is most easily performed. The values required are listed in table 6.1.

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</tbody>
</table>

Table 6.1: Table showing parameters used in COMPASS to convert between JPL Horizons output in ecliptic and cometary orbital plane, obtained from the JPL small body browser [Giorgini et al., 1996]. \(i\) is the inclination of the comet’s orbit, node is the longitude of the ascending node and peri is the argument of perihelion. All quantities are given in degrees in the J2000.0 reference frame.

For the COMPASS simulations representing the Brown et al. [1998] and Rauer et al. [1998] data (i.e. observations 1, 2, 3 and 4) we initially selected the total simulation time based on the consideration of the characteristic lifetime of photoionisation of neutral sodium at 1 AU presented in equation (5.4), chapter 5, but found that a large percentage of the simulated atoms lay outside the slits for these simulations and were therefore not forming a useful part of the output.

In order to rectify this situation the lifetime of atoms within the slit was determined from the initial simulation based on the total simulation time calculated using equation (5.4). The results of this method are given in figure 6.5, which shows the percentage of atoms within the slit for each observation considered at or below a given lifetime. From these plots it was noticed that for observations 1, 2, and 3 the majority of atoms were within a 95% of the maximum lifetime in the slit.

In these cases, the 5% of COMPASS particles with the largest lifetimes may be either high velocity (in which case they are likely to be far from the cometary nucleus and are relatively few so the brightness at that position would be negligible) or they may be low velocity (in which case they are likely to exist within the stagnation region discussed in chapter 2 and are therefore of negligible brightness compared to the large number of atoms present there). In either case the relatively long lifetime means that their brightness is likely to be negligible unless there are large numbers of these atoms.
(which is not the case at the 5% level). Excluding the top 5% where the cutoff threshold was clear, produced significant advantages to computational cost (total simulation time went from over 1 day to hours in all cases meaning convergence could be reached sooner) compared to relatively few disadvantages due to the different weightings used in COMPASS resulting in the minority top 5% lifetime particles within the slit being unlikely to contribute significantly to the final output (see chapter 5). For observations 1, 2 and 3 the cutoff threshold was therefore chosen to be 95%, but for observation 4 the dropoff in lifetime within the slit was smooth so the full 100% of the maximum lifetime within the slit was used as the total simulation time in this case. The total simulation times selected for COMPASS based on this approach for each Brown et al. [1998] and Rauer et al. [1998] data set is listed in table 7.1.

![Cutoff threshold used for each of the intensity profile simulations considered in this chapter. For observations 1, 2 and 3 a 95% cutoff threshold was used for simulating atoms within the artificial slit as the dropoff was abrupt. For observation 4, the dropoff in particle lifetime was smooth and therefore the maximum age of atoms within the slit was considered.](image)

**Figure 6.5:** Cutoff threshold used for each of the intensity profile simulations considered in this chapter. For observations 1, 2 and 3 a 95% cutoff threshold was used for simulating atoms within the artificial slit as the dropoff was abrupt. For observation 4, the dropoff in particle lifetime was smooth and therefore the maximum age of atoms within the slit was considered.

### 6.5.2 COMPASS Output Plot Parameters

For comparison with the intensity profiles produced by Brown et al. [1998] and Rauer et al. [1998], we use the artificial slit parameters and resolution given in table 6.3. The artificial slit dimensions were chosen using the the length of slit recorded in the measurement and the maximum width of slit available. The maximum slit width was chosen to minimise computational cost, whilst ensuring the simulation realistically represented the observation. Artificial slit angles were calculated using the Sun–comet line, and two artificial slit angles are used on 16 April 1997 for comparison with the Rauer et al. [1998] data because the observations were taken both parallel and perpendicular to the Sun–comet line.
<table>
<thead>
<tr>
<th>Parameter</th>
<th>Obs 1</th>
<th>Obs 2</th>
<th>Obs 3</th>
<th>Obs 4</th>
</tr>
</thead>
<tbody>
<tr>
<td>Figure Reference</td>
<td>6.1</td>
<td>6.2</td>
<td>6.3</td>
<td>6.4</td>
</tr>
<tr>
<td>Observation Date</td>
<td>8 Apr 1997</td>
<td>14 Mar 1997</td>
<td>16 Apr 1997</td>
<td>16 Apr 1997</td>
</tr>
<tr>
<td>Observation Time (UT)</td>
<td>03:30</td>
<td>03:51</td>
<td>20:22</td>
<td>21:19</td>
</tr>
<tr>
<td>Observation Distance (AU)</td>
<td>0.923</td>
<td>0.956</td>
<td>0.956</td>
<td>0.957</td>
</tr>
<tr>
<td>Simulation Date</td>
<td>8 Apr 1997</td>
<td>14 Mar 1997</td>
<td>16 Apr 1997</td>
<td>16 Apr 1997</td>
</tr>
<tr>
<td>Simulation Time (UT)</td>
<td>03:30</td>
<td>03:51</td>
<td>20:22</td>
<td>21:19</td>
</tr>
<tr>
<td>Simulation Distance (AU)</td>
<td>0.923</td>
<td>0.956</td>
<td>0.956</td>
<td>0.956</td>
</tr>
<tr>
<td>Effective Simulation Duration (hours)</td>
<td>14.5</td>
<td>20.0</td>
<td>15.0</td>
<td>63.0</td>
</tr>
<tr>
<td>Effective Simulation Duration Threshold</td>
<td>95%</td>
<td>95%</td>
<td>95%</td>
<td>100%</td>
</tr>
<tr>
<td>Light Travel Time Correction (mins)</td>
<td>13</td>
<td>12</td>
<td>14</td>
<td>14</td>
</tr>
</tbody>
</table>

Table 6.2: Table detailing the observations of comet Hale-Bopp considered in this study.

### 6.5.3 Convergence in COMPASS

In order to implement COMPASS in a self consistent way that facilitates comparison with observational data, it is necessary to ensure that the results of COMPASS converge. The approach implemented in order to obtain a meaningful degree of convergence in COMPASS is discussed generally in chapter 5. The threshold for convergence was set at $T = 10\%$, using the criterion for convergence in equation (5.15), chapter 5. The values of $T$ produced by the results we consider to be converged, the number of sodium atom particles produced per timestep required for convergence and the number of timesteps required for convergence for each of the simulations discussed in this chapter are given in table 6.4.

*Brown et al. [1998]* and *Rauer et al. [1998]* Convergence In order to ensure that the intensity profiles produced by COMPASS were a true representation of the simulation result we again used the convergence criterion previously discussed in equa-
Table 6.3: Table detailing artificial slit parameters used in COMPASS output plots to facilitate comparison with Brown et al. [1998] and Rauer et al. [1998] observations. True slit parameters (used to take observations) are listed as unstarred quantities, whereas the slit parameters chosen for COMPASS simulations are listed as starred quantities. Res* indicates the artificial one dimensional slit resolution chosen.

<table>
<thead>
<tr>
<th>Date</th>
<th>Obs</th>
<th>Width</th>
<th>Length</th>
<th>Width*</th>
<th>Length*</th>
<th>Angle* (degrees)</th>
<th>Res*</th>
</tr>
</thead>
<tbody>
<tr>
<td>14 March</td>
<td>2</td>
<td>0.3-13.0 arcsec</td>
<td>5.5 arcmin</td>
<td>13.0 arcsec</td>
<td>5.5 arcmin</td>
<td>-345.3°</td>
<td>101</td>
</tr>
<tr>
<td>8 April</td>
<td>1</td>
<td>0.2-1.2 arcsec</td>
<td>6.0 arcmin</td>
<td>1.2 arcsec</td>
<td>6.0 arcmin</td>
<td>-39.8°</td>
<td>51</td>
</tr>
<tr>
<td>16 April</td>
<td>3,4</td>
<td>0.14-22.6 arcsec</td>
<td>4.0 arcmin</td>
<td>22.6 arcsec</td>
<td>4.0 arcmin</td>
<td>-55.3° (/el), 34.6° (perp)</td>
<td>101</td>
</tr>
</tbody>
</table>

Table 6.4: Table showing the converged number of timesteps and the converged number of sodium atom particles per timestep for the simulations of comet Hale-Bopp discussed in this chapter. The level of convergence of each set of simulations is also shown. It was not always possible to achieve the desired $T = 10$ level of convergence as the timestep results diverged quickly.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Obs 1</th>
<th>Obs 2</th>
<th>Obs 3</th>
<th>Obs 4</th>
</tr>
</thead>
<tbody>
<tr>
<td>Converged Number of Particles (particles)</td>
<td>13600</td>
<td>850</td>
<td>425</td>
<td>3400</td>
</tr>
<tr>
<td></td>
<td>6.3</td>
<td>6.9</td>
<td>7.3</td>
<td>7.1</td>
</tr>
<tr>
<td>Converged Number of Timesteps</td>
<td>281</td>
<td>1126</td>
<td>1126</td>
<td>9008</td>
</tr>
<tr>
<td></td>
<td>8.0</td>
<td>10.4</td>
<td>9.4</td>
<td>19.5</td>
</tr>
</tbody>
</table>

We desired the threshold for convergence to be set at $T = 10\%$, but this was not always possible for these simulations as the timestep had to be so short and the number of timesteps had to be so large to ensure that sufficient atoms lay within the slit. This caused the result of the simulation to diverge quickly. A larger artificial slit size could rectify this problem, but in trialling this method we found that it significantly changed the dynamics of the neutral sodium atom particles within the slit, as the ratio of atoms inside the collision radius to outside changed dramatically. The issue of divergence effects the timestep convergence, but it has no effect on the convergence of the number of sodium atom particles produced per timestep.

At the point of convergence, increasing the number of atoms is equivalent to decreasing the timestep in the simulation. Furthermore, the more atoms are present within the simulation, the easier it is to distinguish the point at which the simulation converges. Therefore for the COMPASS implementation of the simulation for the Brown et al. [1998] and Rauer et al. [1998] observations we first converge the number of atoms produced per timestep, using a relatively small number of timesteps. We then use the converged number of atoms to converge the number of timesteps, in order to be able to more easily distinguish the point at which the simulations diverge (as typically con-
 Comparison between COMPASS results and Observations for Comet Hale-Bopp (C/1995 O1)

Convergence requires a large number of atoms). We therefore choose the point of timestep convergence to be the point where $T$ is minimised, which for observation 2 and 4 meant that the $T = 10$ criterion was not met (see table 6.4).

Plots showing the number of atoms per timestep and timestep convergence of the artificial image produced by COMPASS are shown in figures 6.6 and 6.7 respectively. n1 indicates a simulation that produced 53 neutral sodium atom particles per timestep, and each subsequent choice of number of neutral sodium atom particles produced per timestep sees it double (i.e. $n_1=53, n_2=106, n_3=212, n_4=425, n_5=850, n_6=1700$). Similarly, timestep interval $i_1$ indicates a simulation that uses 140 intervals over the total length of the simulation, and each subsequent choice of timestep interval sees the number of timesteps double over that range (i.e. $i_1=140$ intervals, $i_2=281$ intervals, $i_3=563, i_4=1126$ intervals etc).

6.6 Comparison between COMPASS results and Observations for Comet Hale-Bopp (C/1995 O1)

We now discuss the outputs of COMPASS simulations of comet Hale-Bopp using the methodology discussed in this chapter and in chapter 5.

Comparison with Brown Intensity Profiles [Brown et al., 1998] The intensity profile produced for comet Hale-Bopp for observation 1 using the COMPASS dust and nuclear sources are shown in figure 6.8. A comparison between the results of
Comparison between COMPASS results and Observations for Comet Hale-Bopp (C/1995 O1)

Figure 6.7: Plot showing the convergence of each of the Brown et al. [1998] and Rauer et al. [1998] Hale-Bopp COMPASS simulation intensity profile plot outputs with number of timestep intervals over total length of simulation in time. i1=140 intervals, i2=281 intervals, i3=563, i4=1126 intervals etc.

COMPASS and the Brown et al. [1998] model for observation 1, which does not include consideration of the orbital motion of the comet (see chapter 4 for more details), is also shown in figure 6.8. In each case the COMPASS models have been scaled such that the maximum intensity at the nucleus position matches the maximum intensity in the model (i.e. 100% relative intensity). From figure 6.8 it is apparent that:

- Ahead of the collision radius on the sunward side of the nucleus, none of the COMPASS sources are able to reproduce the observed emission.
- An increase in intensity on the sunward side of the nucleus within the collision radius is reproduced by the COMPASS nuclear and dust sources.
- An increased region of neutral sodium emission on the sunward side of the nucleus in seen in the data and reproduced by both the Brown et al. [1998] and COMPASS models, but the effect of including orbital motion appears to smooth out the increase in intensity. The smoother increase in intensity seen in COMPASS more accurately reflects the observation.
- The Brown et al. [1998] dust model is greater in intensity ahead of the comet nucleus than at the nucleus position. This behaviour is not seen in any of the COMPASS models.
- The values of intensity on the sunward side of the nucleus within the collision radius are not adequately represented by either COMPASS source, but may be represented by a combination of the two.
- The COMPASS dust model seems to be very similar to the dust intensity on both
the sunward and anti-sunward side of the nucleus within the collision radius.

- The full width half maximum of the neutral sodium emission is approximately equal to that of the output from COMPASS nuclear source, but smaller than the data using the COMPASS dust model.

- The gradients of the neutral sodium and dust emissions are shallow and comparable to the gradients in the nuclear and dust COMPASS models on the anti-sunward side of the nucleus outside the collision radius.

Figure 6.8: Plot comparing the intensity profile produced by the COMPASS dust and nuclear sources, that observed by Brown et al. [1998] and the Brown et al. [1998] models on the same date. The vertical light blue lines indicate the limit of the collision radius. A negative comet nucleus distance indicates a position on the sunward side of the comet nucleus.

Figure 6.9 shows that for both the COMPASS dust and nuclear sources the most important factor affecting the simulated intensity is the number of atoms at that position, and that the brightness effects included act to enhance the increase in intensity inside the collision radius ahead and behind the nucleus thereby broadening the full width half maximum of the simulated emission. The brightness effects have similar effects on both COMPASS sources. The simulations have the same orbital and observational characteristics, and COMPASS particles are produced with the same initial velocity, but the dust and nuclear sources evolve differently because particles are produced in different positions. This result therefore indicates that the differences in velocity during the evolution of the two COMPASS sources is negligible, i.e. that it is the velocity of the sodium atom particle at production that has the largest effect on its subsequent evolution.
Figure 6.9: Plot showing the composition of the intensity profile produced by the COMPASS nuclear source and dust source in the simulation of observation 1. The vertical light blue lines indicate the limit of the collision radius. ‘All’ indicates that all brightness effects have been considered, and ‘Number’ indicates that only the number of neutral sodium atom particles has been considered. All other brightness effects follow the naming conventions given in chapter 5.2.3. A negative comet nucleus distance indicates a position on the sunward side of the comet nucleus.
Comparison with Rauer Intensity Profiles [Rauer et al., 1998] The intensity profile produced for comet Hale-Bopp for observation 2, 3 and 4 using the COMPASS dust and nuclear sources are shown in figures 6.10, 6.12 and 6.15 respectively.

From figure 6.10 it is apparent that:

- Ahead of the collision radius on the sunward side of the nucleus, none of the COMPASS sources are able to reproduce the observed emission.
- An increase in intensity on the sunward side of the nucleus within the collision radius is reproduced by the COMPASS nuclear and dust models.
- The values of intensity on the sunward side of the nucleus within the collision radius are not adequately represented by either COMPASS source, but may be represented by a combination of the two.
- The COMPASS dust model seems to be very similar to the dust intensity on the sunward side of the nucleus seen in the data but the intensity on the anti-sunward side of the nucleus within the collision radius is much larger using the COMPASS dust and nucleus model than observed in the neutral sodium and dust emissions.
- The full width half maximum of the emission is greater in the COMPASS nuclear model than in the data, but smaller than the data in the COMPASS dust model.
- The gradients of the neutral sodium and dust emissions are shallow and comparable to the gradients in the nuclear and dust COMPASS models on the anti-sunward side of the nucleus outside the collision radius.

Figure 6.11 shows that for this observation the limiting brightness effect is ‘Dist2’ (i.e. the decrease in solar intensity with the square of heliocentric distance). As for figure 6.9, the effect of including different brightness effects is independent of the choice of COMPASS source.

From figure 6.12 it is apparently that:

- Ahead of the collision radius on the sunward side of the nucleus, none of the COMPASS sources are able to reproduce the observed emission.
- An increase in intensity on the sunward side of the nucleus within the collision radius is reproduced by the COMPASS nuclear and dust models. However, the neutral sodium emission shows a decrease in intensity that is not observed in COMPASS using either source.
- The values of intensity on the sunward side of the nucleus within the collision radius are not adequately represented by either COMPASS source.
- The COMPASS dust source output is very different to the observed dust distribution.
Comparison between COMPASS results and Observations for Comet Hale-Bopp (C/1995 O1)

Figure 6.10: Plot comparing the intensity profile produced by the COMPASS dust and nuclear sources and that observed by Rauer et al. 1998 on the same date. The vertical light blue lines indicate the limit of the collision radius. A negative comet nucleus distance indicates a position on the sunward side of the comet nucleus.

- The intensity on the anti-sunward side of the nucleus within the collision radius is larger than observed in the data using the COMPASS dust source, but approximately equal to the COMPASS nucleus model.
- The full width half maximum of the emission is greater in the COMPASS nuclear model than in the data, but smaller than the data in the COMPASS nuclear model.
- The gradients of the neutral sodium and dust emissions are shallow and comparable to the gradients in the nuclear and dust COMPASS models on the anti-sunward side of the nucleus outside the collision radius.

Figure 6.13 shows that the limiting brightness factor for simulations of observation 3 is the same as for observation 2 i.e. ‘Dist2’. As for the 6.9 and 6.11, the effect of including different brightness effects is independent of the choice of COMPASS source.

Figure 6.15 shows that the results are very different when considering the neutral sodium emission intensities perpendicular to the Sun–comet line. A schematic of the approximate position of the slit in the simulation is shown in figure 6.14. It can be seen that:

- Inside the collision radius, the qualitative behaviour of both COMPASS sources appears in approximate agreement with the sodium emission observed. An in-
Comparison between COMPASS results and Observations for Comet Hale-Bopp (C/1995 O1)

(a) COMPASS nuclear source

(b) COMPASS dust source

Figure 6.11: Plot showing the composition of the intensity profile produced by the COMPASS nuclear source and dust source in the simulation of observation 2. The vertical light blue lines indicate the limit of the collision radius. ‘All’ indicates that all brightness effects have been considered, and ‘Number’ indicates that only the number of neutral sodium atom particles has been considered. All other brightness effects follow the naming conventions given in chapter 5.2.3. A negative comet nucleus distance indicates a position on the sunward side of the comet nucleus.
Figure 6.12: Plot comparing the intensity profile produced by the COMPASS dust and nuclear sources and that observed by Rauer et al. [1998] on the same date. The vertical light blue lines indicate the limit of the collision radius. A negative comet nucleus distance indicates a position on the sunward side of the comet nucleus.

crease in emission on the left hand side of the comet nucleus is observed using both sources, followed by a more prominent emission on the right hand side of the comet nucleus (i.e. neutral sodium emission is more pronounced in the direction that the comet travels).

- The full width half maximum of the simulated emission is much larger than that observed.
- The emission simulated using the COMPASS nuclear source has a larger full width half maximum than the emission simulated using the COMPASS dust source.

Figure 6.16 shows that the limiting brightness factor for simulations of observation 4 is the same as for observations 2 and 3 i.e. ‘Dist2’. As for the previous simulations in this chapter, the effect of including different brightness effects is independent of the choice of COMPASS source, which was also seen in figures 6.9, 6.11 and 6.13.

6.7 Conclusions

The results presented in this chapter show the importance of using an orbital model of neutral sodium emission, such as COMPASS, particularly in reproducing different features in the leading and trailing sections of the comet’s orbit. The COMPASS
Figure 6.13: Plot showing the composition of the intensity profile produced by the COMPASS nuclear source and dust source in the simulation of observation 3. The vertical light blue lines indicate the limit of the collision radius. ‘All’ indicates that all brightness effects have been considered, and ‘Number’ indicates that only the number of neutral sodium atom particles has been considered. All other brightness effects follow the naming conventions given in chapter 5.2.3. A negative comet nucleus distance indicates a position on the sunward side of the comet nucleus.
sources produce different outputs for each observation, indicating that orbital motion has an effect on the observed intensity of neutral sodium at the comet, even in the small region of comet Hale-Bopp’s orbit considered in these simulations. In particular, COMPASS simulations of observations 2 and 3 give different results, despite being at identical heliocentric distances.

Figure 6.14: Schematic describing the slit orientation used to simulate observation 4, produced as a standard output using COMPASS.

Figure 6.15: Plot comparing the intensity profile produced by the COMPASS dust and nuclear sources and that observed by Rauer et al. [1998] on the same date. The vertical light blue lines indicate the limit of the collision radius. A positive comet nucleus distance indicates a position on the leading side of the comet’s orbit.
Figure 6.16: Plot showing the composition of the intensity profile produced by the COMPASS nuclear source and dust source in the simulation of observation 4. The vertical light blue lines indicate the limit of the collision radius. ‘All’ indicates that all brightness effects have been considered, and ‘Number’ indicates that only the number of neutral sodium atom particles has been considered. All other brightness effects follow the naming conventions given in chapter 5.2.3. A positive comet nucleus distance indicates a position on the leading side of the comet’s orbit.
The perihelion of comet Hale-Bopp occurred on 1 April 1997, therefore observation 2 was taken before perihelion and observations 1, 3 and 4 were taken after perihelion. Pre-perihelion and post-perihelion observations of neutral sodium show different features and for the majority of the simulations presented here, the qualitative behaviour of the emission is reproduced by COMPASS using either source. Therefore the convergence condition \( T = 10 \) appears to produce valid results. Although observation 2 does not meet the condition \( T = 10.4 \), the output is comparable to those produced for observations 1 and 3 and as this is relatively close to \( T = 10 \) we do not believe that this significantly effects the results. However, the large difference in full width half maximum between the simulations and data in observation 4 may also be a result of the simulation not being fully converged.

The change in intensity that results from inclusion of many different brightness effects is small for the observations considered here. In all cases considered in this chapter the limiting factors affecting the final simulated intensity of the emission were either the heliocentric distance of the particle or the number of particles, and if simulating spectra in the future it is likely to be computationally more efficient to neglect the other brightness effects.

The observations of sodium emission presented in this chapter typically show very shallow gradients on the anti-sunward side of the nucleus, which means that it is difficult to objectively judge the validity of COMPASS models at these distances using this data (typically at distances greater than \( 1 \times 10^5 \) km for comet Hale-Bopp during this passage). It is important to consider the gradients instead of the true values in this region because if a combination of sources are to be considered, one might imagine a large combination from a highly localised nucleus source that would dominate the emission immediately surrounding the nucleus (a more localised source was not compatible with COMPASS because of the use of the collision radius parametrisation - see chapter 5). The scaling of the results of the simulations presented in this chapter to a maximum intensity at the nucleus may therefore be irrelevant.

The outputs of the COMPASS and Brown et al. [1998] models give a poor match to the observations on the sunward side of the nucleus in front of the collision radius. This may be a result of how the initial distributions are set up for the dust and nuclear sources. The COMPASS source set up (outlined in chapter 5) is identical to that of Brown et al. [1998], but inclusion of orbital motion is likely to require a larger maximum COMPASS particle production distance.

The full width half maximum of the simulation of observation 4 is much greater than that observed, whereas for observations 2 and 3 it is comparable. This may indicate that the spherical collision radius approximation may not be suitable when looking very close to the cometary nucleus. It was used successfully by Brown et al. [1998] in their model (see chapter 4), but they did not consider observations perpendicular to the Sun–comet line.
6.8 Further Work

Although COMPASS is able to match the qualitative behaviour of observations presented in this chapter, it is unable to match the quantitative behaviour. This may indicate the need for further research into the nature of the source of sodium at comets close to the nucleus, by studying the sodium measurements taken in situ at similar, active comets close to perihelion. COMPASS would also likely benefit from the inclusion of a more realistic dust source originating at the nucleus, which accurately reflects the sunward to anti-sunward asymmetries seen in the dust observations.

Observations 2, 3 and 4 were taken when the comet was at a heliocentric distance of approximately 0.956 AU, whereas observation 1 was taken when comet Hale-Bopp was at a heliocentric distance of 0.923 AU. This difference in heliocentric distance likely resulted in a slight increase in the production rate of the comet, and therefore the collision radius for observation 1 should be slightly larger than for 2, 3 and 4. A study investigating the effect of a variable collision radius could be used to determine its importance.

We also wish to create a velocity map of different regions within the slit to facilitate comparison with the Brown et al. [1998] observation. At each slit position this would be achieved by investigating the velocity distributions at each small region within the slit and fitting a Gaussian profile to the curve to determine the central velocity peak for the neutral sodium atom particles within that segment of the slit. It is likely that this approach will be more sensitive to convergence than the current intensity profile simulations and will therefore require more atoms produced per timestep and therefore the availability of significantly more computational resources.

Modelled behaviour within the collision radius does not always accurately represent the data. This may be the result of the discrete collision radius used in COMPASS and would likely benefit from the inclusion of collisional effects in a more physical, functionally smooth form. If the collision radius approximation is to be used for computational efficiency, it is likely to be more realistic to use a non-spherical collision radius very close to the nucleus. This effect is likely to be negligible at large cometocentric distances.
Chapter 7

Application of COMPASS to Imaging Observations of Comet Hale-Bopp (C/1995 O1)

7.1 Introduction

In this chapter we discuss the application of COMPASS (see chapter 5) to the initial Cremonese et al. [1997b] neutral sodium tail detection image of comet C/1995 O1 Hale-Bopp (henceforth Hale-Bopp). The sodium emission from this comet was studied extensively due to the interest ignited by this image, with various authors attributing their observations to different sources and transient features at the comet (see discussion in chapter 3). These observations were not imaging, but spectroscopy, and are discussed in chapter 6. The aim of this chapter is to reproduce the Cremonese et al. [1997b] image of the neutral sodium tail at comet Hale-Bopp and draw conclusions about the source(s) of sodium at comet Hale-Bopp based on this result. We also wish to extend the model to other images of comets of interest (see chapter 9). Drawing more robust conclusions about the source of sodium in comets more generally is important, although it must be noted that high activity comets like Hale-Bopp are relatively rare and such conclusions may only be used tentatively in practice.

7.2 Aims of this study

Determining the source of sodium at a comet is extremely challenging but as the sum of data available on Hale-Bopp is more than any previously studied comet prior to C/2012 S1 (ISON) (particularly concerning the measurement of sodium emission) it represented an excellent opportunity for research.
In order to draw together the observations of comet Hale-Bopp in a comprehensive manner that can be most easily simulated using COMPASS and allow conclusions to be drawn about the overall behaviour at comet Hale-Bopp, we seek to simulate the sodium measurements analysed by Cremonese et al. [1997b]. For more details on the CoCam instrument see chapter 3.

The Cremonese et al. [1997b] image taken by the CoCam instrument was selected for comparison with COMPASS because it is wide field and therefore simulating this data could provide insight into the distribution of sodium atoms relatively far from the cometary nucleus.

7.3 Observations

In April 1997 a sodium tail was clearly identified at comet Hale-Bopp by Cremonese et al. [1997b]. The initial discovery image obtained using the CoCam wide field imaging instrument on La Palma (using a range of different filters) is reproduced in figure 7.1. Quantitative surface brightnesses were not obtained from the wide field images due to difficulty in calibrating them. We use this image to test COMPASS’s ability to reproduce the relative brightness of neutral cometary sodium atom emission far from the comet nucleus.

![Figure 7.1: Two images of comet Hale-Bopp, spanning 7.4° or 3.1 × 10^7 km at the comet nucleus [Cremonese et al., 1997b]. Left/Right image obtained using narrow band Na/H_2O^+ filter on April 16.9 UT [Cremonese et al., 1997b]. The continuum image has not been subtracted from either image.](image)

7.4 Preparation of the Observations

**Wide field observations** The nature of the CoCam instrument was such that the neutral filter was positioned by hand, making absolute calibration very difficult even if the calibration images (flat field, dark field, flux calibration) were available. For the observation we wish to simulate, calibration images were not available. Therefore we may only compare the morphology of the neutral sodium tail and relative brightness
of these images, and are unable to use them to quantify the absolute brightness of the sodium tail.

In order to directly compare the result of the simulation with the imaging data the image was artificially pixelated onto the same grid as that chosen for the simulation (see chapter 7.5). Pixelation of the CoCam image was achieved by first processing the image using Astrometry.net [Lang et al., 2012] to obtain the celestial (right ascension and declination) coordinates of pixels in the image. The Lang et al. [2012] processed image (proc) is shown plotted in the COMPASS Earth sky plane in figure 7.2. In the left of figure 7.2 the image has not been cropped, but as the vignetting in the image was significant, proc was cropped to the region encompassing the cometary tails (right of figure 7.2) to facilitate comparison with COMPASS.

![Figure 7.2: A diagram showing the result of processing the CoCam image using Astrometry.net [Lang et al., 2012]. Plotted in the COMPASS Earth sky plane, the left image is the direct output as a result of processing using Astrometry.net [Lang et al., 2012] and the right image has been cropped to remove vignetting. Both images displayed have been scaled to the maximum intensity in the cropped image at 100 percent to display the comet correctly without false stretching of the scale due to the bias strip in the uncropped image. The scales have also been set to show from zero to 2.5 percent relative intensity, with any pixels with an intensity greater than 2.5 percent shown in the same manner as those with 2.5 percent relative intensity. This scaling is for visualisation purposes only, and does not represent a fundamental change to the data. The raw data (i.e. 0-100% intensity) and used in the results that follow).](image)

In order to facilitate direct comparison with the output of the model, the CoCam image (in celestial coordinates) must then be transformed such that it lies on the same grid as that used to construct the artificial image used in COMPASS by pixelation. The CoCam images are pixelated onto the COMPASS image grid by summing the values of the CoCam pixels within each COMPASS image grid. This process introduces a uniform artefact into the image, which arises from the observed image pixels lying on a grid that has a different orientation to the artificial image grid, such that some sections of artificial image grid contain more observed image pixels than others. The uniformity of this artefact gives confidence to the uniformity of the artificial image grid, and may be removed by averaging out the effect. The artefact was removed by separating it out from the image by pixellating a uniform image (i.e. one where the pixels have the same...
celestial coordinates as the image being considered, but where the value at each pixel is equal to 1) onto the artificial image grid, and then dividing the pixelated image by the uniform pixelated image. The application of this process to the CoCam image of comet Hale-Bopp is shown in figure 7.3.

An estimate of the background intensity level in the image was then obtained by calculating the median value of a region of the image that was away from the comet. The region selected for this image of comet Hale-Bopp is shown in green in figure 7.4, but the median background estimated was reasonably independent of the region selected. The result was then interpreted on a relative intensity scale, so that the intensity of the brightest part of the neutral sodium emission (i.e. at the nucleus) was 100%. The result of the processing on this image is shown in figure 7.4, with the image on the left showing the result without removal of background approximation. The results in figure 7.4 have been contrast enhanced to make cometary features more easily apparent. This is implemented for the display only, as direct comparison of the pixelated image with the results of COMPASS would not be possible if the image had been contrast enhanced.

Artifacts are seen surrounding the cropped CoCam image and are a result of interpolation where no intensity values were available. As the artefacts do not represent physical emission and are not present within the region occupied by the neutral sodium tail we they are not considered in our analysis or discussed further. The full process required to produce the final CoCam image to be compared with the COMPASS results may be described by:

1. Process image using astrometry.net [Lang et al., 2012].
2. Crop image to remove vignetting and irrelevant regions of data.
3. Pixelate image onto same grid and COMPASS artificial image, and removal of resulting artefact.
4. Remove median background from image.

---

**Figure 7.3:** Example plot showing the result of pixelating the CoCam image of comet Hale-Bopp onto the same grid as that used for COMPASS (A, left), determination of the resulting artefact using a uniform image (B, centre) and its removal (C=A/B, right).
Figure 7.4: Images obtained by pixelating the CoCam image processed using Astrometry.net [Lang et al., 2012] and scaling it so that the brightest intensity value at the nucleus represents 100% relative intensity. The left image shows the result of this process without the removal of the estimated background intensity before the scaling step in the processing, with the region used to estimate the background shown in green. The centre image shows only the region used to estimate the background. The right image shows the result of this process including the removal of estimated background intensity.

7.5 COMPASS Implementation

The general procedures for implementation of COMPASS are discussed in chapter 5. In this chapter we discuss the application of those general procedures facilitate comparison of COMPASS with the observations of comet Hale-Bopp outlined in chapter 7.3 and discussed in detail in chapter 3.

7.5.1 COMPASS Simulation Parameters

The collision radius used in COMPASS for these simulations is \( r_c = 4 \times 10^4 \) km, based on the successful comparison of the Brown et al. [1998] simulation with observational data at 1 AU. This value of collision radius is appropriate for this study because comet Hale-Bopp was at approximately 1 AU during the observation considered in this chapter.

We corrected the date of the observation to be simulated for light travel time to the nearest minute (see chapter 5 for more details) and then used the light travel time corrected observation date and the total time of the simulation calculated using equation (5.4), to run the appropriate dates through the JPL Horizons online database [Giorgini et al., 1996] and to extract the three dimensional positions \((x, y, z, v_x, v_y, v_z)\) of comet Hale-Bopp and the observer at Earth. The orbital parameters of comet Hale-Bopp used in this study are identical to those given in table 6.1.

For the CoCam simulations the start time of the simulations was selected to be 12 days, 19 hours and 21 minutes before the observation date, based on the consideration
of the characteristic lifetime of photoionisation of neutral sodium at 1 AU presented in equation (5.4), chapter 5.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Cremonese et al. [1997b] Image</th>
</tr>
</thead>
<tbody>
<tr>
<td>Figure Reference</td>
<td>7.1</td>
</tr>
<tr>
<td>Observation Date</td>
<td>16 Apr 1997</td>
</tr>
<tr>
<td>Observation Time (UT)</td>
<td>21:08</td>
</tr>
<tr>
<td>Observation Heliocentric Distance (AU)</td>
<td>0.969</td>
</tr>
<tr>
<td>Observation Distance from Earth (AU)</td>
<td>1.538</td>
</tr>
<tr>
<td>Phase Angle (degrees)</td>
<td>39.43</td>
</tr>
<tr>
<td>Field of view (ra and dec)</td>
<td>$6.14 \times 10^7\ km = 12.0^\circ$</td>
</tr>
<tr>
<td>Simulation Date</td>
<td>16 Apr 1997</td>
</tr>
<tr>
<td>Simulation Time (UT)</td>
<td>21:00</td>
</tr>
<tr>
<td>Simulation Distance (AU)</td>
<td>0.956</td>
</tr>
<tr>
<td>Simulation Length (dd:hh:mm)</td>
<td>12:19:21</td>
</tr>
<tr>
<td>Light Travel Time Correction (mins)</td>
<td>14</td>
</tr>
</tbody>
</table>

Table 7.1: Table detailing the observations of comet Hale-Bopp considered in this study.

### 7.5.2 COMPASS Output Plot Parameters

An output simulation of $100 \times 100$ pixels was chosen as most appropriate to facilitate comparison of COMPASS with the Cremonese et al. [1997b] CoCam image, as a higher resolution was too computationally expensive (because in order for a sufficient number of neutral sodium particles in COMPASS to be present within each box on the COMPASS simulation grid a large number of atoms must be within the simulation to produce a converged result) and a significantly lower resolution was also insufficient to establish the morphology of the neutral sodium tail produced by COMPASS.

### 7.5.3 Convergence in COMPASS

In order to implement COMPASS in a self-consistent way that facilitates comparison with observational data, it is necessary to ensure that the results of COMPASS converge. The approach implemented in order to obtain a meaningful degree of convergence in COMPASS is discussed generally in chapter 5. The threshold for convergence was set at $T = 10\%$, using the criterion for convergence in equation (5.15), chapter 5. For the simulation discussed in this chapter, the values of $T$ produced by the results we consider to be converged, the number of sodium atom particles produced per timestep required for convergence and the number of timesteps required for convergence are given in table 8.2.

**CoCam Convergence** Figures 7.5 and 7.6 show the convergence obtained for COMPASS outputs for the CoCam detection image. The threshold, $T = 10\%$, criterion was
### Table 7.2

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Observation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Converged Number of Timesteps</td>
<td>590</td>
</tr>
<tr>
<td>( T ) (timestep)</td>
<td>9.1</td>
</tr>
<tr>
<td>Converged Number of Particles per timestep</td>
<td>850</td>
</tr>
<tr>
<td>( T ) (particles)</td>
<td>8.9</td>
</tr>
</tbody>
</table>

Table 7.2: Table showing the converged number of timesteps and the converged number of sodium atom particles per timestep for the simulations of comet Hale-Bopp discussed in this chapter. The level of convergence of each set of simulations is also shown, for the intensity profile plots it was not always possible to achieve the desired \( T = 10 \) level of convergence as the timestep results diverged quickly.

Selected to ensure the image converged, based on the convergence criterion (equation (5.15), chapter 5). This threshold was chosen based on the scale of the CoCam image and the availability of computational resources. Plots showing the timestep and number of atoms per timestep convergence of the artificial image produced by COMPASS are shown in figures 7.5 and 7.6 respectively. Timestep interval \( i_1 \) indicates a simulation that uses 147 intervals over the total length of the simulation, and each subsequent choice of timestep interval sees the number of timesteps double over that range (i.e. 147 intervals, \( i_2 = 295 \) intervals, \( i_3 = 590 \), \( i_4 = 1180 \) etc). Similarly, \( n_1 \) indicates a simulation that produced 53 neutral sodium atom particles per timestep, and each subsequent choice of number of neutral sodium atom particles produced per timestep sees it double (i.e. \( n_1 = 53 \), \( n_2 = 106 \), \( n_3 = 212 \), \( n_4 = 425 \), \( n_5 = 850 \), \( n_6 = 1700 \)). The initial selection of collision radius determined the initial number of timestep intervals chosen directly, as we selected the timestep interval which would give a corresponding distance step of greater than approximately twice the collision radius to avoid the same unphysical results produced by the inclusion of a the purely nucleus source in an orbital model with a collision radius (see chapter 5). Meaningful convergence was obtained using COMPASS in its current form with the simulation and output plot parameters previously specified, with 590 timestep intervals and 850 particles produced per timestep.

![Figure 7.5](image)

**Figure 7.5:** Plot showing the convergence of the CoCam Hale-Bopp COMPASS simulation plot outputs with number of timestep intervals over total length of simulation in time. \( i_1 = 147 \) intervals, \( i_2 = 295 \) intervals, \( i_3 = 590 \), \( i_4 = 1180 \) etc.
7.6 Comparison between COMPASS results and Observations for Comet Hale-Bopp (C/1995 O1)

We now discuss the outputs of COMPASS simulations of comet Hale-Bopp using the methodology discussed in this chapter and in chapter 5. The results of the converged, light travel time corrected COMPASS simulations for Hale-Bopp at 21:00 16 April 1997 are shown in figure 7.7. The comparison between the pixelated neutral sodium filter image and the artificial image is favourable, with the neutral sodium tail simulated using both the nuclear and dust sources lying approximately on top of the neutral sodium tail in the pixelated image. The additional tail in the pixelated CoCam image is due to the dust tail. The COMPASS nucleus and dust sources presented in this chapter are not capable of reproducing neutral sodium emission that originated in the dust tail.

The results of the converged, light travel time corrected COMPASS simulations for Hale-Bopp at 21:00 16 April 1997 are shown in figure 7.8, where the syndynes have been calculated using the Finson and Probstein [1968] model with the $\beta$ values used
Comparison between COMPASS results and Observations for Comet Hale-Bopp (C/1995 O1) by Cremonese et al. [1997b] (i.e. \(79 \leq \beta \leq 85\), see chapter 8 for in depth discussion of \(\beta\) and the Finson and Probstein [1968] model). The plot shows that this range of \(\beta\) values produces a good agreement with COMPASS and the CoCam image close to the cometary nucleus, but that the models deviate at large cometocentric distances.

Figure 7.8: Plot showing the results of the converged, light travel time corrected COMPASS simulations for the CoCam image of comet Hale-Bopp taken at 21:00 16 April 1997 compared to the artificially pixelated image with the \(\beta\) values used by Cremonese et al. [1997b] overlaid. \(79 \leq \beta < 85\) is shown in green on each plot with \(\beta = 85\) shown in blue. See chapter 8 for more information on the model used to produce these syndynes.

There are five significant factors considered in COMPASS that determine the relative intensity of the COMPASS neutral sodium tail at any position (see chapter 5 for more details):

1. The number of neutral sodium tail particles at that position.
2. The time since each particle was produced.
3. The velocity of each particle.
4. The heliocentric distance of each particle.
5. The distance between each particle and the observer.

Figures 7.9 and 7.10 show the brightness intensity profiles produced by COMPASS as a result of each of these factors for the dust and nuclear COMPASS sources respectively. The brightness effects have the same influence on both sources, as expected as the observational perspective and orbital motion are the same in both simulations. In both cases, the limiting brightness effect is ‘Fraction’, which describes the loss of neutral sodium atoms due to photoionisation.

Figure 7.11 shows reasonably good agreement between the morphology of the neutral sodium tails simulated by COMPASS and the CoCam observation, using both sources. However, there is a small offset between the position of the simulated neutral sodium tail and that in the CoCam image.

As the radius of the Earth is approximately \(6371 \text{ km} = 4.263 \times 10^{-5} \text{ AU}\) and the
Comparison between COMPASS results and Observations for Comet Hale-Bopp (C/1995 O1)

Figure 7.9: Plot showing the different brightness factors that combine to result in the light travel time corrected COMPASS dust source simulation for the CoCam image of comet Hale-Bopp taken at 21:00 16 April 1997 using a constant collision radius. ‘All’ indicates that all brightness effects have been considered, and ‘Number’ indicates that only the number of neutral sodium atom particles has been considered. All other brightness effects follow the naming conventions given in chapter 5.2.3.

Figure 7.10: Plot showing the different brightness factors that combine to result in the light travel time corrected COMPASS nucleus source simulation for the CoCam image of comet Hale-Bopp taken at 21:00 16 April 1997 using a constant collision radius. ‘All’ indicates that all brightness effects have been considered, and ‘Number’ indicates that only the number of neutral sodium atom particles has been considered. All other brightness effects follow the naming conventions given in chapter 5.2.3.
Figure 7.11: Contour plot showing the differences in morphology between the results of the converged, light travel time corrected CoCam image of comet Hale-Bopp taken at 21:00 16 April 1997 (shown in green using the scale on the right) compared to the artificially pixelated image (shown in red using the scale on the left).

The distance between the comet and the Earth at the time of the observation was 1.538 AU, the maximum difference between the true comet position and that simulated (as a result of the simulation origin being taken as the centre of the Earth for simplicity instead of the observer at La Palma) is given by \( \arctan(4.263 \times 10^{-5}/1.538) \), which equates to 5.7 arcsec. This difference is therefore insufficient to explain the observed shift.

Atmospheric refraction may also be a possible cause of the offset between the position of the simulated neutral sodium tail and that in the CoCam image. The astrometric right ascension and declination of the comet based on an observer at La Palma at 21:00 14 April 1997 are 03 41 41.10 and +35 21 40.9 degrees respectively, whereas the apparent right ascension and declination are 03 41 29.39 and +35 21 01.7 degrees respectively (obtained from JPL Horizons [Giorgini et al., 1996]). Therefore a shift of approximate 2 seconds in right ascension and 29 arcseconds in declination is due to refraction by the atmosphere and insufficient to explain the observed shift.

In figure 7.11, both sources appear to produce a neutral sodium tail that is more extended than the CoCam image. On the sunward side of the cometary nucleus the dust source also produces a large excess of neutral sodium emission.

Dust emission from comet Hale-Bopp would also be detected by the orange filter image. Cometary dust grains emit strongly in the orange filter and all features observed in the CoCam image of comet Hale-Bopp may not be a direct result of neutral sodium emission. To compensate for this effect, we only consider the scaling of the COMPASS artificial images produced where the emission is considered to be entirely from neutral cometary sodium, i.e. where the bright pixel lies entirely within the distinct neutral sodium tail.

The orange emission reminiscent of a cometary dust tail that is detected in the CoCam image of comet Hale-Bopp is not reproduced by the COMPASS simulations using any of the appropriate sources. The feature may be entirely a result of the scattering of
solar radiation due to dust particles, but may also result from the release of neutral sodium atoms within the dust tail which requires a different source distribution.

### 7.7 Conclusions

In this chapter we have produced the first fully heliocentric distance and velocity dependent model of wide field image of the neutral sodium tail at comet Hale-Bopp. The results of the COMPASS simulations using the nuclear and dust sources presented show good agreement with the morphology of the processed, pixelated image of comet Hale-Bopp taken by CoCam. The brightness effects are dominated by the loss of neutral sodium by photoionisation for both sources, but both sources produce neutral sodium tails that are more extended than the tail seen in this observation. This may indicate that additional loss processes may be important, or that the use of some parameterisation in COMPASS (e.g. the discrete, spherical collision radius) effectively lengthens the neutral sodium tail simulated.

The CoCam orange filter image, when compared to the ion filter image, shows significant orange emission from the dust tail, which is unaccounted for by the nucleus and dust source distributions used in COMPASS.

### 7.8 Further Work

A comparison between the CoCam image of comet Hale-Bopp and the results of the dust and nuclear COMPASS sources found that the emission is reminiscent of a cometary dust tail. The cometary dust tail itself emits somewhat strongly in the neutral sodium wavelengths, and may therefore be responsible for the entirety of this emission. However, neutral cometary sodium may also be released from the dust tail and begin to form part of the neutral sodium tail observed at this comet. The likelihood of this feature detected being a result of neutral sodium emission or solar radiation scattered by dust is investigated by the Finson and Probstein [1968] model incorporated in COMPASS in chapter 8.

The work presented in this chapter could be extended by introducing an additional loss rate, of the form:

\[ S \propto e^{-t/\tau^*} \quad , \]

where \( \tau^* \) is characteristic time for neutral sodium depletion. \( \tau^* \) would be difficult to determine analytically but a trial and error approach could be adopted to see whether this method produces more appropriate results.
Chapter 8

Application of the COMPASS true dust tail model to relevant observations

8.1 Introduction

In this chapter we discuss the addition of a true dust tail source distribution in COMPASS (see chapter 5), and its application to the Cremonese et al. [1997b] observation of comet Hale-Bopp previously studied in chapter 7. We use a simplistic Finson and Probstein [1968] model to simulate the dust tail of comet Hale-Bopp over the period considered in the COMPASS simulation and investigate whether it is likely that neutral sodium emission could have its source in the cometary dust tail.

8.2 Aims of this study

Initial study of the CoCam image of comet Hale-Bopp presented in chapter 7 suggested that the most likely source of neutral sodium based on this observation was the extended $1/r^2$ source, initially used by Brown et al. [1998] and considered representative of dust and neutral gas outflow from the coma. In order to determine whether a purely dust source is sufficient to explain the neutral sodium emission detected at this comet, in this study we produce a more physical dust source distribution model in COMPASS, based on a simplistic Finson and Probstein [1968] model of a range of dust particles with different $\beta$. This approach provides the ability to test whether the observations are consistent with neutral sodium atoms being produced in the cometary dust tail, and if so which region of the dust tail they are most likely to originate in.

One of the difficulties in determining the source of cometary sodium is that it would
appear initially that sodium produced in the coma is entrained within the gas outflow, and therefore the initial neutral sodium atom velocity distribution caused by the production of neutral sodium in the cometary environment would be lost. In this study we also test whether observations are consistent with the initial velocity of the neutral sodium atoms produced in the cometary dust tail being that of the dust particles in the tail.

8.3 The Finson and Probstein [1968] model as an Input to COMPASS

The Finson and Probstein [1968] model has been successfully used as a means of identifying the age of outbursts in the dust tail, by tracking the position of synodynes and synchrones produced by the model. Modern dust tail models use a similar Monte-Carlo approach to that adopted by COMPASS, but these results are more detailed than is required for our purposes (e.g. Kharchuk et al. [2009]). Therefore in order to reproduce the approximate positions and velocities of dust particles within the tail we use a simplistic Finson and Probstein [1968] approach. The key parameter of a Finson and Probstein [1968] model is the $\beta$ of each individual dust particle, which is defined in equation (1.1). Therefore the evolution of dust particles in this model is achieved using:

$$F_{\text{tot}} = F_{\text{grav}} - F_{\text{rad}}$$  \hspace{1cm} (8.1a)

$$M_p a_{\text{tot}} = F_{\text{grav}} \left(1 - \frac{F_{\text{rad}}}{F_{\text{grav}}} \right)$$  \hspace{1cm} (8.1b)

$$= F_{\text{grav}}(1 - \beta)$$  \hspace{1cm} (8.1c)

where $F_{\text{tot}}$ is the total force acting on the dust particle in the sunward direction, $a_{\text{tot}}$ is the total acceleration acting on the particle and $M_p$ is the mass of the particle. The gravitational force, $F_{\text{grav}}$, acting on a particle of mass, $m$, due to an object of mass, $M$, is defined by Newton’s law of gravitation as:

$$F_{\text{grav}} = \frac{M_p M G}{d^2}$$  \hspace{1cm} (8.2)

where $d$ is the distance between the two objects and $G = 6.6738480 \times 10^{-11} \text{ m}^3\text{kg}^{-1}\text{s}^{-2}$ is the gravitational constant. In our case the object which dominates the gravitational force acting on the dust particles in the comet is the Sun, we therefore use $M = M_S = 1.98892 \times 10^{30} \text{ kg}$. Therefore the total acceleration acting on a dust particle as a result of the gravitational force of the Sun in the simulation is given by:
The Finson and Probstein [1968] model as an Input to COMPASS

\[ a_{tot} = \frac{M_s G}{R^2} (1 - \beta) \], \hspace{1cm} (8.3)

where \( R \) is the heliocentric distance of the particle. As the \( \beta \) distribution of dust particles at comets is unknown (because Finson and Probstein [1968] models have traditionally not been used to estimate dust distributions) therefore we select the maximum, \( \beta_{\text{max}} \), and minimum, \( \beta_{\text{min}} \), \( \beta \) values based on our observation of the cometary dust tail to be considered. We use uniform \( \beta \) distributions in different ranges within the apparent dust tail to simulate the result of a neutral sodium tail produced from different regions of the dust tail.

As in COMPASS, particles are produced with zero cometocentric velocity, but in the dust model we have included no consideration of a collision radius or initial distribution. Instead, all dust particles are produced with a chosen \( \beta \) distribution that does not vary throughout the simulation.

Evolution in the Finson and Probstein [1968] model we have developed for use with COMPASS is implemented in the standard manner, using a selection of different \( \beta \) values that are chosen based on the region of the dust tail we wish to investigate.

The maximum age, \( \text{age}_{\text{max}} \), defines the start of the Finson and Probstein [1968] model to be implemented prior to COMPASS in order to produce a dust tail source of neutral sodium (i.e. the Finson and Probstein [1968] simulation starts at the time \( t - \text{age}_{\text{max}} \), where \( t \) is the start of the original COMPASS simulation). Once a dust particle is produced and evolved, if the condition:

\[ \text{age} > \text{age}_{\text{max}} \], \hspace{1cm} (8.4)

is satisfied then all future evolution of the dust particle’s position is stopped and it is removed from consideration in plotting routines. Dust particles where this condition is true will not be used as input to the COMPASS routine to produce neutral sodium atoms, and therefore this condition also acts as a limit on the range of the dust particle distribution produced at each timestep.

In using the Finson and Probstein [1968] model as an input to COMPASS, the first step is to run and save the approximate positions and velocities of dust particles of different \( \beta \) in the dust tail. This is implemented for each step used in the COMPASS simulation. The COMPASS neutral sodium atom positions and velocities are then assigned randomly based on a \( 1/r^2 \) distribution (where \( r \) is cometocentric distance) of the dust particle positions where equation (8.4) is satisfied.
8.4 Preparation of Observations and COMPASS Implementation

The preparation of the observations for this study is identical to that described in chapter 7. The COMPASS simulation and plotting routines were implemented using the same parameters as described in chapter 7. The additional parameters required for implementation of the dust source are listed in table 8.1. The three ranges of $\beta$ values were selected to assist in the understanding of which type of dust is more likely to be responsible for the formation of a neutral sodium tail. As the dust source model itself produces no brightness distribution, we used a best judgement approach when deciding the most appropriate number of dust particles produced per timestep that would facilitate coverage of the range of dust visible whilst maximising the effective use of computational resources. A constant dust production rate was assumed throughout these simulations.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>High Mass</th>
<th>Medium Mass</th>
<th>All</th>
</tr>
</thead>
<tbody>
<tr>
<td>Maximum Age of Dust (days)</td>
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<td>100</td>
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<tr>
<td>$\beta_{\text{max}}$</td>
<td>0.05</td>
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<tr>
<td>$\beta_{\text{min}}$</td>
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<td>0.001</td>
<td>0.001</td>
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<tr>
<td>Number of Dust Particles per Timestep</td>
<td>100</td>
<td>100</td>
<td>100</td>
</tr>
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</table>

Table 8.1: Table detailing the parameters used to produce a Finson and Proebstein [1968] model for the CoCam image of comet Hale-Bopp. Three different $\beta$ distributions were used to capture different regions of the dust tail.

A converged artificial image for each of the $\beta$ distributions implemented was obtained in the same manner as that used in chapter 7. The criterion for convergence (equation (5.15), chapter 5) was used with a threshold, $T = 10\%$, as discussed in chapter 5, based on the scale of the CoCam image and the availability of computational resources. The values of $T$ produced by the results we consider to be converged, the number of sodium atom particles produced per timestep required for convergence and the number of timesteps required for convergence for each of the simulations discussed in this chapter are given in table 8.2.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>High Mass</th>
<th>Medium Mass</th>
<th>All</th>
</tr>
</thead>
<tbody>
<tr>
<td>Converged Number of Timesteps</td>
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<td>590</td>
<td>590</td>
</tr>
<tr>
<td>T (timestep)</td>
<td>6.8</td>
<td>6.1</td>
<td>6.7</td>
</tr>
<tr>
<td>Converged Number of Particles per timestep</td>
<td>106</td>
<td>425</td>
<td>850</td>
</tr>
<tr>
<td>T (particles)</td>
<td>8.4</td>
<td>8.8</td>
<td>4</td>
</tr>
</tbody>
</table>

Table 8.2: Table showing the converged number of timesteps and the converged number of sodium atom particles per timestep for the simulations of comet Hale-Bopp discussed in this chapter. The level of convergence of each set of simulations is also shown, for the intensity profile plots it was not always possible to achieve the desired $T = 10\%$ level of convergence as the timestep results diverged quickly.
Plots showing the timestep and number of atoms per timestep convergence of the artificial image produced by COMPASS are shown in figures 8.1 and 8.2 respectively. Timestep interval \( i_1 \) indicates a simulation that uses 147 intervals over the total length of the simulation, and each subsequent choice of timestep interval sees the number of timesteps double over that range (i.e. \( i_1 = 147 \) intervals, \( i_2 = 295 \) intervals, \( i_3 = 590 \), \( i_4 = 1180 \) intervals etc). Similarly, \( n_1 \) indicates a simulation that produced 53 neutral sodium atom particles per timestep, and each subsequent choice of number of neutral sodium atom particles produced per timestep sees it double (i.e. \( n_1 = 26 \), \( n_2 = 53 \), \( n_3 = 106 \), \( n_4 = 212 \), \( n_5 = 425 \), \( n_6 = 850 \), \( n_7 = 1700 \)).

**Figure 8.1:** Plot showing the convergence of each of the Hale-Bopp Finson and Probstein [1968] dust tail model COMPASS simulation plot outputs with number of timestep intervals over total length of simulation in time. \( i_1 = 147 \) intervals, \( i_2 = 295 \) intervals, \( i_3 = 590 \), \( i_4 = 1180 \) intervals etc.

**Figure 8.2:** Plot showing the convergence of each of the Hale-Bopp Finson and Probstein [1968] dust tail model COMPASS simulation plot outputs with number of sodium atom particles produced per timestep. \( n_1 = 26 \), \( n_2 = 53 \), \( n_3 = 106 \) etc.
8.5 Comparison between COMPASS results and Observations

Figure 8.3 shows the syndyne plots for each of the different ranges of $\beta$ used in the simulations discussed in this study, as described in table 8.1. The dust tail source labelled ‘All’ dust was selected to map the entirety of the dust tail observed at Hale-Bopp, whereas the other sources were chosen to represent part of the tail. As neutral sodium is a relatively high mass atom (mass number = 23 amu) we expect a source within the larger mass dust grains to produce a better match to the neutral sodium tail.

![Figure 8.3: Syndyne plots showing the ranges of $\beta$ values used for the at the final comet nucleus position in the simulations. The syndynes produced by all $\beta$ values are shown in pink except for $\beta_{\text{max}}$, which is shown in green.](image)

Figure 8.4 shows the plots of relative intensity produced by each of the simulation results for the high mass, medium mass range and all dust included in the relevant simulations. The location of the dominant neutral sodium tail is the same for each simulation and matches the position of the tail simulated in chapter 7 even though no nuclear sources were included, which indicates that even if the neutral sodium originated in the dust tail it rapidly transitions into the dominant neutral sodium tail feature observed (for comet Hale-Bopp from this observational perspective). In each case a secondary tail-like feature was also produced, which roughly coincided with the lightest (highest $\beta$) regions of the dust tail. The transition between the two most prominent regions is negligible in each simulation.

Figure 8.5 shows that the COMPASS dust simulations produce a good fit to the morphology of the neutral sodium tail identified in this observation of comet Hale-Bopp. The COMPASS results also indicate that a secondary neutral sodium tail feature may be present within the cometary dust tail, and that the morphology of this feature depends strongly on the original dust source distribution. Identifying the morphology of the secondary neutral sodium tail may therefore be key to characterising the type of dust from which the sodium was released.
8.6 Conclusions

In this chapter we have presented the results of the use of a simplistic dust tail source within COMPASS to simulate the observation of comet Hale-Bopp initially considered in chapter 7. The results show that, as for chapter 7, the dominant brightness effect is the loss of neutral sodium by photoionisation. They also broadly reproduce the dominant neutral sodium tail in the CoCam images, but also show secondary features, whose morphology depends on the $\beta$ distribution of dust selected for the simulation and appears to coincide with the lowest mass region of dust simulated.

As the Finson and Probstein [1968] model has not been used in this manner previously no information is currently available on the $\beta$ distributions present within cometary dust tails. However, the simulations presented in this chapter (using uniform $\beta$ distributions) suggest that the presence of secondary neutral sodium tails (or other, similar features
immediately around the main cometary dust tail) may indicate that a fraction of the neutral sodium observed originated within the cometary dust tail.

8.6.1 Further Work

The work presented in this chapter is promising, but in order to generalise the result we must first apply the COMPASS dust tail source models to other high activity comets other than Hale-Bopp and then to other comets with different characteristics.

The Finson and Probstein [1968] model used to simulate a dust tail source using COMPASS is simplistic and computationally inexpensive but more sophisticated Monte-Carlo dust tail simulations exist that may produce more accurate results. The modular design of COMPASS makes it easy to add additional functionality such as this.
Figure 8.6: Plot showing the different brightness factors that combine to result in the light travel time corrected COMPASS source simulation for the CoCam image of comet Hale-Bopp taken on 21:00 16 April 1997 using a constant collision radius and the high mass dust tail source. ‘All’ indicates that all brightness effects have been considered, and ‘Number’ indicates that only the number of neutral sodium atom particles has been considered. All other brightness effects follow the naming conventions given in chapter 5.2.3.

Figure 8.7: Plot showing the different brightness factors that combine to result in the light travel time corrected COMPASS source simulation for the CoCam image of comet Hale-Bopp taken on 21:00 16 April 1997 using a constant collision radius and the medium mass dust tail source. ‘All’ indicates that all brightness effects have been considered, and ‘Number’ indicates that only the number of neutral sodium atom particles has been considered. All other brightness effects follow the naming conventions given in chapter 5.2.3.
Figure 8.8: Plot showing the different brightness factors that combine to result in the light travel time corrected COMPASS source simulation for the CoCam image of comet Hale-Bopp taken on 21:00 16 April 1997 using a constant collision radius and the all dust tail source. ‘All’ indicates that all brightness effects have been considered, and ‘Number’ indicates that only the number of neutral sodium atom particles has been considered. All other brightness effects follow the naming conventions given in chapter 5.2.3.
Chapter 9

Application of COMPASS to comets observed by LASCO

9.1 Introduction

The COMPASS model was initially applied to comet Hale-Bopp in order to understand the formation of a strong neutral sodium tail feature that had been observed in detail through both spectroscopy and imaging (see chapters 6 and 7 respectively for more information). The application of COMPASS to the images of comet Hale-Bopp was particularly successful, so we now consider images of neutral sodium tails at different comets in order to more fully understand the formation of neutral sodium tails at comets, and to gather more evidence on the source of neutral sodium in comets. Comets like Hale-Bopp are relatively rare, and therefore we must consider other data sets to understand whether the results of COMPASS may be applied more generally.

It had been noted (e.g. by Geraint Jones and Hugh Osborn [Jones and Osborn, 2015]) that some near-Sun comets observed by the LASCO coronagraph on the SOHO spacecraft (see chapter 3 for more details SOHO and LASCO) appear to display significant neutral sodium features based on a comparison between images taken using the orange, blue and clear filters.

Near-Sun comets are objects that have extremely small perihelion distances (less than 0.307 AU, the perihelion of Mercury’s orbit, based on the convention adopted in Jones et al. [2016]) and behave very differently to comets like Hale-Bopp. More discussion of previous near-Sun comet observations is presented in chapter 2.6.

As the conditions for comets within the LASCO field of view are somewhat different to comets like Hale-Bopp, these observations provided a useful test to the generality of COMPASS in addition to facilitating a comparison between the neutral sodium tails observed at comets at different heliocentric distances. It also allow us to study how the neutral sodium tail features observed at near-Sun comets differ from those observed at
more typical comets with larger perihelia.

9.2 Aims of this study

The LASCO images of comet McNaught, NEAT and Hyakutake considered in this study were taken on different dates, when the comets were at different heliocentric distances. Therefore they provide a good test for the robustness of COMPASS at different heliocentric distances.

The neutral sodium tail of comet McNaught had previously been observed by Snodgrass et al. [2008] and Leblanc et al. [2008], therefore it is considered extremely likely that the neutral sodium tail like feature observed in the SOHO/LASCO image of comet McNaught is indeed the result of neutral sodium emission.

The observation of comet McNaught also provides an excellent initial test for the ability of COMPASS to successfully reproduce features observed in the LASCO field of view because the planet Mercury is also present within the image. The exosphere of Mercury emits strongly in the sodium D line wavelengths (see chapter 1.2.1) and therefore is very bright in the LASCO orange filter, which provides an additional source of verification for the validity of the alterations of observational perspective implemented in COMPASS. We consider that the distinct neutral-sodium-tail-like feature present in the LASCO orange filter image of comet McNaught is likely to be the result of neutral sodium emission based on a comparison with a blue filter image taken at a similar time.

Following the verification of COMPASS provided by comparison with the comet McNaught LASCO images, we next consider the observation of comet NEAT as again orange and blue filter images are available. Both comet NEAT and comet McNaught have similar relative Sun–SOHO–comet positions at the date of the observation, except that the comets are on the opposite sides of the Sun as observed from SOHO (see figure 9.16), therefore similar COMPASS procedures should produce similar results for both comets.

The neutral sodium tail like feature speculated at comet Hyakutake is less likely to be confirmed as neutral sodium emission than those at comets McNaught and NEAT because only the clear filter image is available, and therefore we consider this comet third.

In comparing the results of COMPASS for all observations of near-Sun comets observed by LASCO where neutral sodium tail like features have been observed this study aims to identify whether these features are consistent with neutral sodium emission. Taken as a whole it is hoped that this study will resolve whether near-Sun comets produce neutral sodium tails by the same processes that resulted in the neutral sodium tail at comet Hale-Bopp and if the neutral sodium source distribution is similar.
<table>
<thead>
<tr>
<th>Parameter</th>
<th>McNaught</th>
<th>NEAT</th>
<th>Hyakutake</th>
</tr>
</thead>
<tbody>
<tr>
<td>Perihelion Date</td>
<td>12 Jan 2007</td>
<td>18 Feb 2003</td>
<td>1 May 1996</td>
</tr>
<tr>
<td>Perihelion Distance (AU)</td>
<td>0.170</td>
<td>0.099</td>
<td>0.230</td>
</tr>
<tr>
<td>Observation Date</td>
<td>14 Jan 2007</td>
<td>19 Feb 2003</td>
<td>3 May 1996</td>
</tr>
<tr>
<td>Heliocentric Distance (AU)</td>
<td>0.188</td>
<td>0.119</td>
<td>0.243</td>
</tr>
<tr>
<td>Distance from SOHO (AU)</td>
<td>0.810</td>
<td>1.000</td>
<td>1.217</td>
</tr>
<tr>
<td>Phase Angle (degrees)</td>
<td>148.03</td>
<td>76.70</td>
<td>22.79</td>
</tr>
<tr>
<td>Field of view</td>
<td>$9.0 \times 10^6$ km = 3.538°</td>
<td>$9.0 \times 10^6$ km = 3.520°</td>
<td>$9.0 \times 10^6$ km = 3.452°</td>
</tr>
<tr>
<td>Inclination (degrees)</td>
<td>77.8369</td>
<td>81.7059</td>
<td>124.9228</td>
</tr>
<tr>
<td>Longitude of Ascending Node (degrees)</td>
<td>267.4147</td>
<td>64.08844</td>
<td>188.04522</td>
</tr>
<tr>
<td>Argument of Perihelion (degrees)</td>
<td>155.9749</td>
<td>152.16967</td>
<td>130.1741</td>
</tr>
</tbody>
</table>

Table 9.1: Table detailing the designations and key orbital parameters of the LASCO comets discussed in this study. Orbital parameters were obtained from the JPL horizons database with respect to the J2000.0 frame of reference [Giorgini et al., 1996].

### 9.3 Observations

Near-Sun comets do not always display typical comet features such as comae, dust tails, and ion tails but in the comets considered in this study these features were present, which indicates their high activity levels. The presence of typical cometary features in the comets in this study were crucial to identifying distinct features that could potentially be neutral sodium tails. Many near-Sun comets are speculated to possess neutral sodium tails that overlap other, more prominent cometary features, such as the dust tail or ion tail. In such cases neutral sodium tails may be identified by subtraction of the images taken with the relevant filters (e.g. orange filter image minus blue filter image) but due to the rapid movement of these comets near to perihelion and their dynamic natures this method is challenging and likely to introduce errors. Therefore observations where neutral cometary sodium tails are apparently distinct are preferred and focused on in this study. Table 9.3 outlines the observations of comets C/2006 P1 (McNaught), C/2002 V1 (NEAT) and C/1996 B2 (Hyakutake) considered by this study.

All images selected for this study were taken post-perihelion, which may indicate a preferential bias in the detection of neutral sodium tails before perihelion images were considered but no neutral sodium tails were observed there. This is likely to be due to increased production rates and favourable viewing geometries post-perihelion that results in cometary features being more likely to separate from the dust tail after perihelion and therefore makes distinct neutral sodium tails more likely to be observed.

Diagrams showing the orbital motion of each comet considered in this study are shown in figures 9.1a, 9.1b and 9.1c. We now discuss each of the observations considered in this study in detail.
(a) Plot showing the orbit of comet McNaught. Comet McNaught moves from upper left to the lower left segment of orbit indicated by the blue line.

(b) Plot showing the orbit of comet NEAT. Comet NEAT moves from upper left to the lower left segment of orbit indicated by the blue line.

(c) Plot showing the orbit of comet Hyakutake. Comet Hyakutake moves from left to the right segment of orbit indicated by the blue line.

**Figure 9.1:** Orbital plots of comets McNaught, NEAT and Hyakutake produced using JPL’s Small Body Browser (part of the horizons database) [Giorgini et al., 1996]. The light blue segment of the comets orbit indicates that it is above the ecliptic plane, and the dark blue segments indicate regions where the orbital of the comet is below the ecliptic plane. White lines indicate the orbits of the planets, with green labeled points indicating their positions on the dates shown.
Observations

Figure 9.2: Images of comet McNaught in orange (above) and blue (below) filters of SOHO/LASCO C3. The sodium tail is clearly apparent in the orange filter image and is separate from both the ion and dust tails. Modified from [Jones and Osborn, 2015].

Comet McNaught (C/2006 P1) Figure 9.2 shows images of comet McNaught taken using the orange and blue filters on SOHO/LASCO C3. This again highlights the effective detection of a sodium tail (distinct from ion and dust tails) by a comparison of the images produced in different spectral bands. Again the neutral sodium tail is clearly visible in the orange filter image. Both images show bright spikes due to saturation of the detector.

Comet NEAT (C/2002 V1) Comet C/2002 V1 was discovered by the Near Earth Asteroid Tracking telescope in Hawaii [Helin et al., 1997]. Figure 9.3 shows the images of comet NEAT taken using the same instrument on SOHO as McNaught, but in this instance both the clear and orange filter images are available, so the sodium tail position can be determined by comparison of the primary features present in both images. The clear filter image shows a bright spike to the bottom left hand corner of the image. This is due to saturation of the detector.

Comet Hyakutake (C/1996 B2) Originally there was no sodium tail discovered at comet Hyakutake. However, with the publicity of the sodium tail discovery at Hale-Bopp the data was re-analysed and some authors suggested a sodium tail was present at Hyakutake, even that potentially two tails were visible (identical to the case at Hale-Bopp) [Cremonese, 1999; Mendillo et al., 1998]. Unfortunately this research was not developed further at the time and there are no current publications on an observed sodium tail structure at Hyakutake. The sodium D line emission is observed in the
plasma tail spectrum of comet Hyakutake as a weak feature blended with $H_2O^+$ and $CO^+$ on 1996 March 24:38 UT [Wyckoff et al., 1999].

Figure 9.4 shows an image of Hyakutake taken by SOHO/LASCO C3 using the clear filter. In these data an apparent split in the ion tail is visible. As no orange filter image was taken at the time the results remain unclear, but as there is no reason an ion tail should split in this way it is likely that a sodium tail was observed at Hyakutake. Successful modelling will be critical to analysis of this assumption.

9.4 Preparation of the Observations

The images of these comets taken by LASCO, obtained from SOHO Science Archive [Osuna et al., 2010] in FITS file format, were all processed in the same manner for direct comparison with COMPASS. The four processing steps were:
1. Calibrate LASCO level 0 FITS files to LASCO level 1, using the Solarsoft software developed by Freeland and Handy [1998].

2. Use Solarsoft to translate the raw pixel data into celestial coordinates (right ascension and declination) based on an origin at the SOHO spacecraft.

3. Pixelate each image onto the same grid as the COMPASS artificial image, and remove the artefacts introduced by this step.

4. Construct and subtract a suitable minimum background image (by processing each of the background images in the same way, sigma clipping the result and taking the minimum), to remove the corona.

The SOHO/LASCO images considered in this chapter are ‘level 1’ FITS files. They have been constructed from the ‘level 0.5’ FITS files that have been minimally processed from the original spacecraft data stream (i.e. into FITS format, with solar north at the top of the image) and are available from NASA [2013]. Level 0.5 images have units of DN (digital number of counts) and may be processed to level 1 images (calibrated images with units of mean solar brightness), using the IDL Solarsoft software, which uses processing described by Morrill et al. [2006]. Processing to level 1 images using Solarsoft consists of (in order):

1. Subtraction of offset bias (a positive voltage applied to LASCO’s CCD to ensure that it never reads a negative voltage).

2. Multiplication of the exposure time by the ‘exposure correction factor’ to find the true exposure time, and then dividing the bias subtracted image by this value.

3. Multiplication by the vignetting function, which corrects for the optics of the telescope (i.e. occulting disk and supporting arm).

4. Replacing any missing blocks of data by extrapolation.

5. Subtraction of stray light.

6. Application of correction for geometric distortion (which removes the variation of the angular size of a pixel over the field of view).

7. Multiplication by distortion corrected mask containing the occulter, pylon and outer edge of the field of view.

More detail about each processing step is available in Morrill et al. [2006].

LASCO observes sunlight scattered by electrons in the corona, with the signal integrated over the line of sight. It does not directly observe emission (even cometary emission will be scattered throughout the corona), and so no absolute measurements of cometary emission may be calculated from LASCO data without the use of complex models of coronal scattering that are currently unavailable. However, if it is assumed that the relative amount of scattering is approximately constant for the relatively small
fields of view considered in this study (9 \times 10^6 \text{ km} \text{ by} 9 \times 10^6 \text{ km} \text{ at the comet in each case}), then the relative brightnesses of different sections of the cometary tails observed in the level 1 LASCO images considered in this chapter facilitate the best available comparison with the results of COMPASS.

Solarsoft was also essential in facilitating comparison between the artificial image produced by COMPASS and the LASCO data, as it allowed the celestial coordinates of the images to be calculated. SOHO’s primary function is to study the Sun, therefore the routines implemented in Solarsoft do not fully consider the three dimensional nature of cometary tails present within the LASCO field of view when transforming to other desired reference frames (e.g. celestial coordinates based at Earth). Therefore in order to avoid potential perspective issues we maintain the origin of the LASCO image at the position of the SOHO spacecraft when the image was taken in the J2000 ecliptic reference frame. To facilitate comparison with COMPASS we only transform the initial image to ecliptic celestial coordinates (with SOHO at the origin). We use SPICE Kernels to obtain the position of SOHO, adapted IDL software written by Karl Battams to perform the transformation to the J2000 ecliptic reference frame with the origin at the SOHO spacecraft and IDL software adapted from that written by Geraint Jones to perform the conversion into ecliptic celestial coordinates.

The calibrated LASCO image in celestial coordinates must then be transformed such that it lies on the same grid as that used to construct the artificial image using COMPASS, in order to facilitate direct comparison with the output of the model. The resolution of images produced by COMPASS is limited by computational resources (as the higher the resolution, the more COMPASS particles are required to achieve convergence), but in reality the resolution of the LASCO images discussed in this chapter is only slightly greater than that simulated. The LASCO images are pixelated onto the COMPASS image grid by summing the values of the LASCO pixels within each COMPASS image grid, as previously discussed in chapter 7.4. An example showing the application of this process to the LASCO C3 image of comet McNaught considered in the chapter is shown in figure 9.5. This process was applied to every image considered in this chapter, including all images used to construct the background images.

A suitable background image was constructed from each comet image based on the method used by Knight [2008], but with some notable exceptions. Knight [2008] studied fast moving comets, the majority of which were destroyed during perihelion passage. Knight [2008] therefore used the median of two images prior to the passage of the comet and two images after its passage (and where an even number of images was used, the value taken was the mean of the two central values, using IDL’s ‘even’ keyword with the median routine), but close in time (no more than 24 hours apart) to ensure that the corona was not dramatically different to when the comet was observed. All of the images from which the background image was constructed were checked to ensure they were free from background stars, planets and anomalies (such as cosmic rays) and they
ensured that the same telescope configuration was used in the images that were used to construct the background images.

However, for the LASCO observations considered in this thesis the comets moved relatively slowly through the field of view, the field of view often changes throughout the passage of the comet (as a subframe of the C3 field of view is used), the solar wind conditions change during the observation and the instrumental setup, including the choice of filter, was not repeated for some time following the observations being taken. Therefore for our observations it was not possible to choose background images that did not include the comet in the field of view, and so more background images were included. Table 9.2 shows the images that were used to construct the background images for each comet observation.

In order to remove the majority of the comet signal from the background, we perform kappa-sigma clipping on each of the images to be included in the calculation of the background (including the primary neutral sodium tail detection image considered for the simulation). Kappa-sigma clipping is used to remove high intensity signals with sharp boundaries (see Foundation [2016] for more information), by removing any pixels whose value, $V$, does not meet the following condition:

$$\text{med} - \kappa \sigma < V < \text{med} + \kappa \sigma ,$$  \hspace{1cm} (9.1)

where \text{med} is the median value of the pixels in the image, \(\sigma\) is the standard deviation and \(\kappa\) is a weighting factor. The kappa-sigma clipped images used to construct the background images for each comet observation considered in this chapter and the final, median background images are shown in figures 9.6, 9.7 and 9.8. As it was difficult to completely remove the comet from the background images, we do not use the median value following clipping to estimate the background. Instead, we estimate a minimum
### Table 9.2: Table detailing the images used to construct the background image for each comet observation [Osuna et al., 2010].

<table>
<thead>
<tr>
<th>Parameter</th>
<th>McNaught (Orange filter images)</th>
<th>NEAT (Orange filter images)</th>
<th>Hyakutake (Clear filter images)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Observation Date</td>
<td>14 Jan 2007</td>
<td>19 Feb 2003</td>
<td>3 May 1996</td>
</tr>
<tr>
<td>Observation Time (UT)</td>
<td>16:18:04</td>
<td>12:18:05</td>
<td>13:30:17</td>
</tr>
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<td>Background Image 1B Date</td>
<td>14 Jan 2007</td>
<td>19 Feb 2003</td>
<td>3 May 1996</td>
</tr>
<tr>
<td>Background Image 1B Time (UT)</td>
<td>09:17:33</td>
<td>06:05:30</td>
<td>04:48:47</td>
</tr>
<tr>
<td>Background Image 2B Date</td>
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<td>19 Feb 2003</td>
<td>3 May 1996</td>
</tr>
<tr>
<td>Background Image 2B Time (UT)</td>
<td>11:17:04</td>
<td>08:05:23</td>
<td>06:19:01</td>
</tr>
<tr>
<td>Background Image 3B Date</td>
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<td>19 Feb 2003</td>
<td>3 May 1996</td>
</tr>
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<td>08:32:16</td>
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</tr>
<tr>
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<td>19 Feb 2003</td>
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</tr>
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<td>Background Image 2A Time (UT)</td>
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<td>Background Image 3A Date</td>
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<td>19 Feb 2003</td>
<td>3 May 1996</td>
</tr>
<tr>
<td>Background Image 3A Time (UT)</td>
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<td>Background Image 4A Date</td>
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<td>19 Feb 2003</td>
<td>3 May 1996</td>
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<td>20 Feb 2003</td>
<td>3 May 1996</td>
</tr>
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<td>Background Image 5A Time (UT)</td>
<td>02:17:05</td>
<td>00:05:52</td>
<td>21:38:03</td>
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</table>
Figure 9.6: Plot showing the sigma clipping of each of the background images for the observation of comet McNaught. In table 9.2, images A-E correspond to background images B1-B5, images F-J correspond to background images A1-A5 and image K corresponds to the observation under consideration. A kappa value of 0.39 was used for images A-H and K. Kappa values of 0.07, 0.07, 0.07, 0.015, 0.015, 0.03, 0.03, 0.04, 0.03, 0.03 and 0.02 were used for images A-K respectively. Plot L shows the resulting background image, obtained by taking the median values of images A-K.

background from the minimum values remaining to ensure that no cometary signal is removed.

Although the background images produced using this approach are not always truly representative of the background (e.g. in some cases a planet was present in the comet observation image, which could not be subtracted as background using this approach), for comets McNaught and NEAT the neutral sodium tail was therefore sufficiently far from these features that it did not affect the validity of these results.

The background image constructed for comet Hyakutake using this method is not representative of the background in the immediate vicinity of the observed neutral sodium tail, and obscures this feature due to the presence of the comet in the background images (see figure 9.8). It was very difficult to remove enough of the comet in the background images of Hyakutake without also removing the corona. This is likely due to the Hyakutake image being taken using a clear filter, resulting in comet boundary that is less sharp than for comets McNaught and NEAT. Monthly, minimum background images are available for clear filter LASCO C3 images, but unfortunately the field of view of these images is such that for that epoch they do not overlap with the neutral sodium tail observed at comet Hyakutake (see figure 9.10). Therefore, instead we use the median value of two, comet free regions in the background estimate image (image L in figure 9.8) in the vicinity of the neutral sodium tail, shown in figure 9.11.
Figure 9.7: Plot showing the sigma clipping of each of the background images for the observation of comet NEAT. In table 9.2, images A-E correspond to background images B1-B5, images F-J correspond to background images A1-A5 and image K corresponds to the observation under consideration. Kappa values of 0.2, 0.2, 0.2, 0.2, 0.2, 0.2, 0.7, 0.7 and 0.2 were used for images A-K respectively. Image L shows the resulting background image, obtained by taking the median values of images A-K.

Figure 9.8: Plots showing the sigma clipping of each of the background images for the observation of comet Hyakutake. In table 9.2, images A-E correspond to background images B1-B5, images F-J correspond to background images A1-A5 and image K corresponds to the observation under consideration. Kappa values of 1.0, 1.0, 1.0, 0.5, 0.1, 0.1, 0.05, 0.05, 0.05 and 0.2 were used for images A-K respectively. Image L shows the resulting background image, obtained by taking the median values of images A-K.
Figure 9.9: Plot showing result of the subtraction of the estimated background image from the comet Hyakutake image considered for comparison with COMPASS. The plot shows the result of removing the background median constructed as shown in figure 9.8. No neutral sodium tail is apparent, but the ion tail may still be seen to the right of the comet nucleus.

Figure 9.10: Plot showing the relative positions of the standard median background images closest to the observation of comet Hyakutake and the COMPASS field of view relevant to this observation (shown in pink). The positions of the median images dated 8 April 1996 and 20 May 1996 are shown in orange and green respectively.
Figure 9.11: Plot showing result of the subtraction of the estimated median background from the comet Hyakutake image considered for comparison with COMPASS. The left plot shows the regions selected to calculate an appropriate median from the constructed background image in green, and the centre plot shows only these regions. The right plot shows the result of subtracting the median of these regions from the image of comet Hyakutake. A neutral sodium tail is visible in this image, in contrast with figure 9.9 where it has been removed by the subtraction.

Figure 9.12: Plot showing final results of the processing of the observations of comets McNaught (left), NEAT (centre) and Hyakutake (right) to facilitate comparison with COMPASS.

The final, fully processed, background subtracted images for each comet image considered in this chapter are shown in figure 9.12. The neutral sodium tail is apparent in each image and they are each on the same grid as the relevant COMPASS simulations, facilitating direct comparison. Minor processing effects are introduced in the top left quadrant of the comet McNaught image (resulting from edge effects in images A-C) and top right quadrant of the comet NEAT image (resulting from kappa-sigma clipping that was unable to remove the comet completely), but these effects do not occur in the vicinity of the neutral sodium tail under consideration and may therefore be neglected in this study.

9.5 COMPASS Implementation

The general procedures for implementation of COMPASS are discussed in chapter 5. In this section we discuss the application of those general procedures to facilitate direct comparison of the results of COMPASS with the observations of comets McNaught,
### Table 9.3: Table detailing the designations and key orbital parameters of the LASCO comets discussed in this study. Orbital parameters were obtained from the JPL horizons database [Giorgini et al., 1996]

<table>
<thead>
<tr>
<th>Parameter</th>
<th>McNaught</th>
<th>NEAT</th>
<th>Hyakutake</th>
</tr>
</thead>
<tbody>
<tr>
<td>Observation Date</td>
<td>14 Jan 2007</td>
<td>19 Feb 2003</td>
<td>3 May 1996</td>
</tr>
<tr>
<td>Observation Time (UT)</td>
<td>16:18:04</td>
<td>12:18:05</td>
<td>13:30:17</td>
</tr>
<tr>
<td>Heliocentric Distance at Observation (AU)</td>
<td>0.1876</td>
<td>0.118839</td>
<td>0.242881</td>
</tr>
<tr>
<td>Simulation Date</td>
<td>14 Jan 2007</td>
<td>19 Feb 2003</td>
<td>3 May 1996</td>
</tr>
<tr>
<td>Simulation Time (UT)</td>
<td>16:18</td>
<td>12:18</td>
<td>13:30</td>
</tr>
<tr>
<td>Simulation Distance (AU)</td>
<td>0.1873</td>
<td>0.118841</td>
<td>0.242883</td>
</tr>
<tr>
<td>Simulation Length (dd:hh:mm)</td>
<td>00:11:49</td>
<td>00:04:44</td>
<td>00:19:49</td>
</tr>
<tr>
<td>Light Travel Time Correction (mins)</td>
<td>8</td>
<td>9</td>
<td>11</td>
</tr>
<tr>
<td>Converged Number of Timesteps</td>
<td>1600</td>
<td>1600</td>
<td>800</td>
</tr>
<tr>
<td>Converged Number of Particles per timestep</td>
<td>625</td>
<td>625</td>
<td>625</td>
</tr>
</tbody>
</table>

NEAT and Hyakutake outlined in chapter 9.3 and discussed in detail in chapter 3.

### 9.5.1 COMPASS Simulation Parameters

The implementation of COMPASS for the three LASCO comets in this study has some similarities with the approach adopted for comet Hale-Bopp. The orbital parameters used in COMPASS for the comets in this study are given in table 9.3.

We corrected for light travel time in the same manner as that discussed for comet Hale-Bopp (see chapter 7). Correction for light travel time between comet and observer is more important for the comets in this study because they move quickly through the LASCO field of view. If light travel time is neglected, the position of the comet nucleus predicted by COMPASS does not align with that observed by LASCO (which was not a significant issue for the CoCam image of comet Hale-Bopp). Light travel time correction is calculated in COMPASS to the nearest minute using an iterative approach as discussed in chapter 5.2.1.

As for the simulations of the neutral sodium tail at comet Hale-Bopp, the total COMPASS simulation times for the observations of each comet in this study are listed in table 9.3 (calculated using equation (5.4), see chapter 5.2.1 for more details on this method). The total simulation times were calculated assuming that the heliocentric distance of the comet was that at the time of the observation, which produces longer simulation times than necessary for all the comets in this study as they were observed post perihelion (i.e. moving away from the Sun).

The small heliocentric distances of the comets in this study required a very different COMPASS implementation for calculating the collision radius than that used for comet Hale-Bopp. The general approach used is discussed in chapter 5 and the collision radii used at the relevant heliocentric distances to the comets in this study are shown in figure 9.13.
9.5.2 COMPASS Output Plot Parameters

The parameters chosen for the COMPASS artificial plots for the comets in this study are given in table 9.4. These values were selected based on a consideration of the availability of computational resources, sufficient resolution to facilitate useful comparison and the ability to attain a sufficient level of convergence.

The SOHO spacecraft orbits in a halo orbit around L1 and therefore has a small offset from the L1 position. This offset is significant enough to change the apparent comet nucleus position in the artificial LASCO field of view produced by COMPASS, therefore it is crucial that the exact position of SOHO is used when calculating the transformation required to produce the artificial LASCO image. We therefore use a combination of JPL Horizons [Giorgini et al., 1996] LASCO positions and relevant SPICE Kernels (where Horizons ephemeris data is not available) as the COMPASS artificial image origin.

9.5.3 Convergence in COMPASS

For the imaging results a robust result was obtained in the same manner as that of the comet Hale-Bopp simulations, i.e. using the criterion for convergence for the image simulations discussed in chapter 5. The threshold, $T = 10$, was chosen as the convergence criterion of the results in this study (see equation (5.15), chapter 5) based on the scale of the LASCO images and the availability of computational resources. Plots showing the timestep and number of atoms per timestep convergence of the artificial image pro-
Table 9.4: Table detailing the plot parameters used to generate the artificial LASCO plots in COMPASS. The size and offset of the fields of view are given in the angular form and in km as projected onto the sky plane at the comet’s distance.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>McNaught</th>
<th>NEAT</th>
<th>Hyakutake</th>
</tr>
</thead>
<tbody>
<tr>
<td>Right Ascension (RA) Grid Size in Pixels</td>
<td>100</td>
<td>100</td>
<td>100</td>
</tr>
<tr>
<td>Declination (Dec) Grid Size in Pixels</td>
<td>100</td>
<td>100</td>
<td>100</td>
</tr>
<tr>
<td>Field of view (RA and Dec)</td>
<td>$3.6^\circ = 9.0 \times 10^6$ km</td>
<td>$3.6^\circ = 9.0 \times 10^6$ km</td>
<td>$3.4^\circ = 9.0 \times 10^6$ km</td>
</tr>
<tr>
<td>Offset from Solar Centre (RA)</td>
<td>$-2.0^\circ = -0.5 \times 10^7$ km</td>
<td>$-6.7^\circ = -1.7 \times 10^7$ km</td>
<td>$3.5^\circ = -0.9 \times 10^7$ km</td>
</tr>
<tr>
<td>Offset from Solar Centre (Dec)</td>
<td>$-2.0^\circ = -0.5 \times 10^7$ km</td>
<td>$-2.3^\circ = -0.6 \times 10^7$ km</td>
<td>$5.0^\circ = 1.3 \times 10^7$ km</td>
</tr>
</tbody>
</table>

Produced by COMPASS are shown in figures 9.14 and 9.15 respectively. Timestep interval $i_1$ indicates a simulation that uses 400 intervals over the total length of the simulation, and each subsequent choice of timestep interval sees the number of timesteps double over that range (i.e. $i_1=400$ intervals, $i_2=800$ intervals, $i_3=1600$, $i_4=3200$ intervals etc). Similarly, $n_1$ indicates a simulation that produced 156 neutral sodium atom particles per timestep, and each subsequent choice of number of neutral sodium atom particles produced per timestep sees it double (i.e. $n_1=156$, $n_2=312$, $n_3=625$, $n_4=1250$).

**Figure 9.14:** Plot showing the convergence of each of the LASCO comet COMPASS simulation plot outputs with number of timestep intervals over total length of simulation in time. $i_1=400$ intervals, $i_2=800$ intervals, $i_3=1600$, $i_4=3200$ etc.
9.6 Comparison between COMPASS results and comets observed by LASCO

Diagrams showing the orbital motion period considered for each comet in this study are shown in figures 9.16c, 9.16a and 9.16b, in section 9.3. The principle reason to produce an orbital model of cometary sodium like COMPASS, is to allow for differences in geometry of the observation and evolution. Therefore although we implement COMPASS in the same manner for each LASCO comet in this study, it is important to consider the unique character of their orbits when considering the varying appearance of the neutral sodium tail in each of these cases. Despite the difference in the orbits and observational perspectives between these comets, the number of timesteps and particles required to achieve convergence in COMPASS simulations are remarkably similar.

The first objective for COMPASS was to provide the information needed to deduce whether the features observed in the orange filter LASCO images of these comets were in fact neutral sodium tails. To understand whether this was likely to be the case we first produced plots which overlaid the position of neutral sodium atoms expected from COMPASS on the calibrated, processed LASCO image. These results are shown in figures 9.17, 9.22 and 9.27, and indicate a clear correlation between the expected neutral sodium tail position from COMPASS and the neutral sodium tail-like feature observed by LASCO. In the case of comet Hyakutake (figure 9.27), no orange filter images were available (the neutral sodium tail feature was identified by an apparent, unexplained splitting of the ion tail, see chapter 9.3) and so the neutral sodium tail feature is more difficult to identify. However, the candidate neutral sodium tail feature still appears to align with the expected position from COMPASS and therefore is consistent with neutral sodium emission.
Comparison between COMPASS results and comets observed by LASCO

(a) Plot showing the orbit of comet McNaught relevant to the COMPASS simulation of the observation of this comet discussed in table 9.3.

(b) Plot showing the orbit of comet NEAT relevant to the COMPASS simulation of the observation of this comet discussed in table 9.3.

(c) Plot showing the orbit of comet Hyakutake relevant to the COMPASS simulation of the observation of this comet discussed in table 9.3.

Figure 9.16: Plot showing the orbits of comets McNaught, NEAT and Hyakutake over the periods considered in the relevant simulations. The cometary orbits are indicated by the solid, thick black lines and the projections of these orbit onto the sides of the box plot are shown for reference by three dashed lines on each plot. The orange circles indicate the final position of the comet relevant to the observation simulated, the green circles indicate the position of SOHO/LASCO at the time of the observation (roughly in the ecliptic plane at $z=0$) and the pink circles indices the position of the Sun in the ecliptic (at $(0,0,0)$).

9.6.1 Comet McNaught

Figure 9.17 shows the initial result for a simple COMPASS implementation of comet McNaught. This result has not been converged, but it shows the positions of particle
Comparison between COMPASS results and comets observed by LASCO

produced in COMPASS for this comet over the range of the simulation, and indicates a good match between the neutral sodium tail position observed by LASCO C3 and that produced by COMPASS.

![Figure 9.17](image)

**Figure 9.17:** Plot showing the LASCO orange filter image of comet McNaught with the contrast adjusted to make the neutral sodium tail feature more apparent (left) and the result of a simple COMPASS simulation of the neutral sodium tail overlaid on this image (right). The COMPASS result presented here has not been converged, and uses four hundred timesteps over the simulation time range and ten sodium atoms produced per timestep. The COMPASS simulations use a constant number of atoms per timestep and a variable collision radius, but as the heliocentric distance is always less than the McNaught estimate the distance (see chapter 9.5 for more details) it is effectively constant at 50,000km. The position of Mercury is indicated by an orange triangle in the right hand plot, indicating a high level of accuracy produced by the transformations to the LASCO C3 field of view produced by COMPASS.

The relative intensity of the neutral sodium emissions produced by the COMPASS sources is shown in figure 9.18, and a direct comparison with the LASCO data using contour plots is shown in figure 9.19. These plots show that the COMPASS dust source simulation produces a much broader region of neutral sodium emission than the nuclear source close to the cometary nucleus. The dust source also shows a much more extended neutral sodium emission further from the nucleus, which is clearly not observed in the LASCO C3 image. However, both sources show approximate agreement with the pixelated LASCO C3 image for the morphology of the neutral sodium tail.

Figures 9.20 and 9.21 show the brightness factors affecting the simulated neutral sodium tail image for the observation of comet McNaught, using the nuclear and dust sources respectively. As seen for the observations of comet Hale-Bopp, the brightness effects have similar effects on the overall brightness using both sources. In both sources the dominant brightness factor is the ‘Fraction’ effect, which describes the loss of neutral sodium emission due to photoionisation with a characteristic photoionisation lifetime that is very short at small heliocentric distances.
Comparison between COMPASS results and comets observed by LASCO

Figure 9.18: Plot showing the results of the converged, light travel time corrected COMPASS simulations for the LASCO C3 image of comet McNaught taken at 16:18:04 on 14 January 2007 compared to the artificially pixelated image.

Figure 9.19: Contour plot showing the results of the converged, light travel time corrected COMPASS simulations for the LASCO C3 image of comet McNaught taken at 16:18:04 on 14 January 2007 compared to the artificially pixelated image. Using a constant collision radius.

9.6.2 Comet NEAT

Figure 9.22 shows the initial result for a simple COMPASS implementation of comet NEAT. As for the previous discussion of comet McNaught, this result has not been converged, but it shows the positions of particle produced in COMPASS for this comet over the range of the simulation, and again indicates a good match between the expected neutral sodium tail position based on the LASCO C3 image and that produced by COMPASS.

The relative intensity of the neutral sodium emissions produced by the COMPASS sources is shown in figure 9.23, and a direct comparison with the LASCO data using contour plots is shown in figure 9.24. Again the results of both sources show a broad agreement with the position of the neutral sodium tail observed in the LASCO image, but it is difficult to pick out the neutral sodium tail in the LASCO image as it does not significantly stand out from the background. This is partly the result of the blocks within the image, which are the result of compression of the orange images for transmission to the ground.
Comparison between COMPASS results and comets observed by LASCO

Figure 9.20: Plot showing the different brightness factors that combine to result in the light travel time corrected COMPASS nuclear source simulation for the LASCO C3 image of comet McNaught taken at 16:18:04 on 14 January 2007 using a constant collision radius. ‘All’ indicates that all brightness effects have been considered, and ‘Number’ indicates that only the number of neutral sodium atom particles has been considered. All other brightness effects follow the naming conventions given in chapter 5.2.3.

Figure 9.21: Plot showing the different brightness factors that combine to result in the light travel time corrected COMPASS dust source simulation for the LASCO C3 image of comet McNaught taken at 16:18:04 on 14 January 2007 using a constant collision radius. ‘All’ indicates that all brightness effects have been considered, and ‘Number’ indicates that only the number of neutral sodium atom particles has been considered. All other brightness effects follow the naming conventions given in chapter 5.2.3.
Comparison between COMPASS results and comets observed by LASCO

Figure 9.22: Plot showing the LASCO orange filter image of comet NEAT with the contrast adjusted to make the neutral sodium tail feature more apparent (left) and the result of a simple COMPASS simulation of the neutral sodium tail overlaid on this image (right). The COMPASS result presented here has not been converged, and uses four hundred timesteps over the simulation time range and ten sodium atoms produced per timestep. The COMPASS simulations use a constant number of atoms per timestep and a variable collision radius, but as the heliocentric distance is always less than the McNaught estimate the distance (see chapter 9.5 for more details) it is effectively constant at 50,000km.

Figure 9.23: Plot showing the results of the converged, light travel time corrected COMPASS simulations for the LASCO C3 image of comet NEAT taken at 12:18:05 on 19 February 2003 compared to the artificially pixelated image.

Figures 9.25 and 9.26 show the brightness factors affecting the simulated neutral sodium tail image for the observation of comet NEAT, using the nuclear and dust sources respectively. As for the observation of comet McNaught, the dominant brightness factor is the ‘Fraction’ effect, which describes the loss of neutral sodium emission due to photoionisation with a characteristic photoionisation lifetime that is very short at small heliocentric distances.

9.6.3 Comet Hyakutake

Figure 9.27 shows the initial result for a simple COMPASS implementation of comet Hyakutake. As for the previous discussion of comets McNaught and NEAT, this result has not been converged, but shows the positions of particles produced in COMPASS for
Comparison between COMPASS results and comets observed by LASCO

Figure 9.24: Contour plot showing the results of the converged, light travel time corrected COMPASS simulations for the LASCO C3 image of comet NEAT taken at 12:18:05 on 19 February 2003 compared to the artificially pixelated image. Using a constant collision radius.

Figure 9.25: Plot showing the different brightness factors that combine to result in the light travel time corrected COMPASS dust source simulation for the LASCO C3 image of comet NEAT taken at 12:18:05 on 19 February 2003 using a constant collision radius. ‘All’ indicates that all brightness effects have been considered, and ‘Number’ indicates that only the number of neutral sodium atom particles has been considered. All other brightness effects follow the naming conventions given in chapter 5.2.3.

this comet over the range of the simulation. Again, a good match is observed between the expected neutral sodium tail position based on the LASCO C3 image and that produced by COMPASS.

The relative intensity of the neutral sodium emissions produced by the COMPASS sources for comet Hyakutake are shown in figures 9.28 and 9.30, and direct comparisons with the LASCO data are shown in the contour plots in figures 9.29 and 9.31. It is difficult to distinguish the neutral sodium tail from the background, but these plots again show that COMPASS is able to reproduce the approximate position of the neutral
Comparison between COMPASS results and comets observed by LASCO

Figure 9.26: Plot showing the different brightness factors that combine to result in the light travel time corrected COMPASS nuclear source simulation for the LASCO C3 image of comet NEAT taken at 12:18:05 on 19 February 2003 using a constant collision radius. ‘All’ indicates that all brightness effects have been considered, and ‘Number’ indicates that only the number of neutral sodium atom particles has been considered. All other brightness effects follow the naming conventions given in chapter 5.2.3.

Figure 9.27: Plot showing the LASCO clear filter image of comet Hyakutake with the contrast adjusted to make the neutral sodium tail feature more apparent (left) and the result of a simple COMPASS simulation of the neutral sodium tail overlaid on this image (right). The COMPASS result presented here has not been converged, and uses four hundred timesteps over the simulation time range and ten sodium atoms produced per timestep. The COMPASS simulations use a constant number of atoms per timestep and a variable collision radius described in chapter 9.5.

sodium tail observed, but that the COMPASS dust source produces a much broader neutral sodium tail than that seen by LASCO, especially close to the nucleus. The nuclear source would appear to most closely represent what is observed at the comet in this case.

Figures 9.32, 9.33, show the brightness factors affecting the simulated neutral sodium
Comparison between COMPASS results and comets observed by LASCO

Figure 9.28: Plot showing the results of the converged, light travel time corrected COMPASS simulations for the LASCO C3 image of comet Hyakutake taken at 13:30:17 on 3 May 1996 compared to the artificially pixelated image. Using a variable collision radius.

Figure 9.29: Contour plot showing the results of the converged, light travel time corrected COMPASS simulations for the LASCO C3 image of comet Hyakutake taken at 13:30:17 on 3 May 1996 compared to the artificially pixelated image. Using a variable collision radius.

Figure 9.30: Plot showing the results of the converged, light travel time corrected COMPASS simulations for the LASCO C3 image of comet Hyakutake taken at 13:30:17 on 3 May 1996 compared to the artificially pixelated image. Using a constant collision radius.

tail image for the observation of comet NEAT, using the nuclear and dust sources respectively, using a variable collision radius. Figures 9.34 and 9.35 show the same
Comparison between COMPASS results and comets observed by LASCO

Figure 9.31: Contour plot showing the results of the converged, light travel time corrected COMPASS simulations for the LASCO C3 image of comet Hyakutake taken at 13:30:17 on 3 May 1996 compared to the artificially pixelated image. Using a constant collision radius.

result, using a constant collision radius. As for the other observations discussed in this chapter, the dominant brightness factor is the ‘Fraction’ effect, which describes the loss of neutral sodium emission due to photoionisation with a characteristic photoionisation lifetime that is very short at small heliocentric distances.

Figure 9.32: Plot showing the different brightness factors that combine to result in the light travel time corrected COMPASS dust source simulation for the LASCO C3 image of comet Hyakutake taken at 13:30:17 on 3 May 1996 using a variable collision radius. ‘All’ indicates that all brightness effects have been considered, and ‘Number’ indicates that only the number of neutral sodium atom particles has been considered. All other brightness effects follow the naming conventions given in chapter 5.2.3.

A plot of the difference between the COMPASS results for the comet Hyakutake simulations using variable and constant collision radii for the two sources is shown in figure 9.36. It shows that for this observation of comet Hyakutake, the effect of including a variable collision radius acts to concentrate the neutral sodium emission. In this case
Comparison between COMPASS results and comets observed by LASCO

**Figure 9.33:** Plot showing the different brightness factors that combine to result in the light travel time corrected COMPASS nuclear source simulation for the LASCO C3 image of comet Hyakutake taken at 13:30:17 on 3 May 1996 using a variable collision radius. ‘All’ indicates that all brightness effects have been considered, and ‘Number’ indicates that only the number of neutral sodium atom particles has been considered. All other brightness effects follow the naming conventions given in chapter 5.2.3.

**Figure 9.34:** Plot showing the different brightness factors that combine to result in the light travel time corrected COMPASS dust source simulation for the LASCO C3 image of comet Hyakutake taken at 13:30:17 on 3 May 1996 using a constant collision radius. ‘All’ indicates that all brightness effects have been considered, and ‘Number’ indicates that only the number of neutral sodium atom particles has been considered. All other brightness effects follow the naming conventions given in chapter 5.2.3.
Comparison between COMPASS results and comets observed by LASCO

Figure 9.35: Plot showing the different brightness factors that combine to result in the light travel time corrected COMPASS nuclear source simulation for the LASCO C3 image of comet Hyakutake taken at 13:30:17 on 3 May 1996 using a constant collision radius. ‘All’ indicates that all brightness effects have been considered, and ‘Number’ indicates that only the number of neutral sodium atom particles has been considered. All other brightness effects follow the naming conventions given in chapter 5.2.3.

the variable collision radius is smaller than the constant collision radius used, and as the collision radius is directly related to the width of the neutral sodium tail (see figure 5.2) a narrower sodium tail results from using a variable collision radius to simulate neutral sodium at this comet using these parameters.

Figure 9.36: Difference image plot comparing the results of the converged, light travel time corrected COMPASS simulations for the LASCO C3 image of comet Hyakutake taken at 13:30:17 on 3 May 1996 using a variable and constant collision radius (constant minus variable).
9.7 Conclusions

The COMPASS simulation results presented in this chapter show a good match to the neutral sodium tail position shown in images taken using LASCO C3, despite the difficulties removing the background corona that were especially prevalent in the preparation of the clear filter image of comet Hyakutake. This indicates that the physical principles contained within COMPASS are broadly accurate, but highlights the need for a better characterisation of the neutral sodium source distribution at near-Sun comets in particular. As no COMPASS simulations considered in this chapter include a variation in production rate, the differences in the morphologies of the neutral sodium tails simulated are at least in part the result of the observational perspective and orbital motion of the comet (shown in figure 9.16). The results presented here do not rule out the possibility of a real variations in the production rate of neutral sodium, but do indicate that orbital motion should not be neglected when modelling neutral cometary sodium observations at near-Sun comets.

In all simulations presented in this chapter, the dominant brightness effect was the loss of neutral sodium emission due to photoionisation of neutral sodium, as the characteristic lifetime of neutral sodium is very short at the small heliocentric distances considered here. This result emphasises the importance of correctly characterising the loss rates of neutral sodium at small heliocentric distances.

The COMPASS dust source consistently produced an emission that was too extended to successfully reproduce the neutral sodium tail observed by LASCO, which may be the result of the scale of its initial setup (see chapter 5 for more details) but may also indicate that a $1/r^2$ source does not effectively characterise dust production at such small heliocentric distances.

All COMPASS simulation results are too bright at the nucleus. The nucleus position should contain a large proportion of continuum emission so it is especially troubling that the neutral sodium emission simulated should exceed the total emission in that region. This may be the result of image saturation there (NEAT and McNaught images show saturation spikes), but as the Hyakutake image did not show significant saturation there remains a need to focus on neutral sodium production close to the comet, which was identified as a key area of future research in chapter 6. If the surplus of bright sodium at the nucleus in the COMPASS model is not a result of instrumentation, then it may indicate that the majority of neutral sodium emission is not produced at the cometary nucleus for near-Sun comets.
9.8 Further Work

Although COMPASS has been reasonably effective at characterising the morphology of the neutral sodium tails considered in this chapter, there are many studies that could be carried out to improve the understanding of the dependence of the final simulation result on the input parameters. In particular, it may be important to consider:

- The effect of variation of collision radius.
- The effect of different scales of $1/r^2$ dust source distribution.
- The effect of varying characteristic photoionisation lifetime.
- Whether sublimation of neutral sodium should be incorporated in the source distribution for near-Sun comets. Neutral sodium is known to sublimate in near Sun comets (the heat of sublimation of neutral sodium is approximately 25,000 cal/mol [Sekanina and Kracht, 2014]), and it may be important to consider how this may affect any source distribution produced.

Three observations of neutral sodium tails seen by the LASCO C3 coronagraph were discussed in this chapter, but there are other opportunities to consider neutral sodium tail measurements from space-based instrumentation.

Comet C/2012 S1 (ISON) was observed by LASCO in 2013. Unfortunately comet ISON did not survive its perihelion passage, but some pre-perihelion observations may indicate the presence of a neutral sodium tail. No distinct neutral sodium tail was observed following initial viewing of the data, but this may be because it coincides with the dominant dust tail and could possibly be extracted by comparison between images taken using the blue, orange and clear filters on LASCO. There may also be other LASCO comet images where suitable processing may allow identification of neutral sodium tail-like features. In all cases, appropriate COMPASS simulations would help to identify the likely morphology of a neutral sodium tail.

![Image](image.png)

Figure 9.37: C2 orange filter image showing interesting features in Kreutz sungrazer, comet C/2008 K4. The tail structure on the left is possibly a neutral sodium tail, while the one on the right may be a dust tail.
Furthermore, observations of comets using the LASCO C2 coronagraph often display very strong orange emission, considered to be indicative of neutral sodium [Battams and Knight, 2015]. An example of an observation potentially of interest is shown in figure 9.37. It is currently unknown whether neutral sodium emission is responsible for these features, and COMPASS may provide a suitable method by which this assumption may be tested. However, the implementation of COMPASS would have to be somewhat more complex in order produce the relevant simulations that could explain these observations. In particular, the simple method used to calculate the total COMPASS simulation time used in this study produces accurate COMPASS results because the comets in this study were observed post-perihelion. However for pre-perihelion observations, where the heliocentric distance of the observation is smaller than the heliocentric distance of the comet at the beginning of the simulation, this method would produce a total simulation time that is insufficient to reproduce the neutral sodium tail observed. This is especially true for comets with extremely small perihelia, such as those observed by the LASCO C2 coronagraph, as their heliocentric distances change rapidly and many do not survive perihelion passage. In such cases an iterative approach is required to calculate the total COMPASS lifetime necessary:

1. Calculate the total simulation time, $t_1$, based on the heliocentric distance of the comet at the time of the observation, $t_{\text{obs}}$.
2. Calculate the heliocentric distance of the comet at $t_{\text{obs}} - t_1$, and then use this distance to calculate the new total simulation time, $t_2$.
3. Calculate the heliocentric distance of the comet at $t_{\text{obs}} - t_2$, and use this distance to calculate the new total simulation time, $t_3$ ...

where the correct total simulation time is reached when subsequent steps produce the same total simulation time to an error appropriate to the given set of simulations (e.g. to the nearest minute is expected to be sufficient for a LASCO C2 COMPASS simulation).

COMPASS could also be adapted to simulate other neutral tails (such as that thought to be produced by iron) to help improve our understanding of interesting features such as that identified by Fulle et al. [2007] in STEREO heliospheric images of comet McNaught.
Chapter 10

Concluding Remarks

In this chapter we present an overall summary of the work presented throughout this thesis, focusing on the development of the first fully heliocentric distance and velocity dependent neutral cometary sodium tail model, COMPASS, that has been developed by the author (see chapter 5). In order to understand the validity of COMPASS, we apply the model to a variety of spectroscopic and wide field imaging observations of different comets. The results of these applications are discussed in chapters 6, 7, 8 and 9. A summary of these results and the overall conclusions that may be drawn from them is presented in chapter 10.1. Finally we look at the possibilities for continuation of this work and highlight potential directions for future work in chapter 10.2.

10.1 Summary and Conclusions

Comets are pristine remnants of solar system formation and therefore understanding their composition allows insights into how our solar system formed in such a way that it can sustain a planet capable of supporting human life. With current technology comets are only observable when they become active. The challenge is therefore to determine the original composition and structure of a comet, which would enable information about the material and conditions present at the formation of the Solar System to be gathered, from the often dramatic and transient features observed when comets are active.

The work presented in this thesis sought to understand the formation and evolution of neutral sodium features in comets, and in doing so to better understand the formation of the solar system. Neutral sodium emission is typically bright in active comets, and therefore relatively easy to detect even if the column density is low. Neutral sodium emission has also been identified in planetary systems, such as the Moon, Mercury and at Jupiter’s Moon Io (see chapter 1 for more details). In these cases neutral sodium emission has been used as an indicator of chemical and physical processes. In order
to apply a similar approach to the study of the cometary environment it is necessary to understand the source(s) of neutral sodium in comets, which have not been well identified to date, primarily due to the unintuitive motion of cometary sodium that results from varying Swings/Greenstein effects with different viewing geometries and cometary orbital positions (see chapter 2.2 for more details).

In order to be able to understand the neutral cometary sodium emission features observed at a variety of comets, the author has developed the first fully heliocentric distance and velocity dependent neutral cometary sodium tail model that can be easily adapted to different comets, observation times and viewing geometries. The details of this model, known as COMPASS, are discussed in chapter 5. The author has tested its validity by applying COMPASS to a series of spectroscopic and imaging observations of comet Hale-Bopp at different times (chapters 6, 7 and 8), and to the study of a relatively new group of comets with neutral sodium features: near-Sun comets observed using the LASCO coronagraph (chapter 9).

A distinct neutral sodium tail was initially observed at Hale-Bopp by Cremonese et al. [1997b], which was then studied extensively by other individuals. In chapter 6 we use COMPASS to simulate the spectroscopic observations of comet Hale-Bopp taken by Brown et al. [1998] and Kawakita and Fujii [1998]. COMPASS is able to reproduce the qualitative behaviour of the spectroscopic emission, but no individual source using the standard COMPASS implementation is a more consistent match to the data. As COMPASS uses the same source distributions as the Brown et al. [1998] model, it is perhaps surprising that the results do not produce a better match to the Brown et al. [1998] data (but this may be the result of an error in their initial distribution setup [Brown and Jones, 2004]). The inclusion of orbital motion effects makes it difficult to converge COMPASS on the scales required for this simulation, so we next look at imaging results. In chapter 7 we apply COMPASS to the Cremonese et al. [1997b] wide field image of comet Hale-Bopp taken by CoCam. The results show good agreement with the morphology of the neutral sodium tail but that it is too intense far from the nucleus, possibly suggesting additional loss mechanisms to those considered here. The final comet Hale-Bopp study in this thesis is presented in chapter 8. In this chapter we use a simplistic dust tail source (based on the Finson and Probstein [1968] model) with different, uniform $\beta$ distributions to investigate the result of a neutral sodium source within the dust tail of comet Hale-Bopp. The results show the production of a primary neutral sodium tail (as observed in the wide field image of comet Hale-Bopp taken by Cremonese et al. [1997b]) and a secondary neutral sodium tail feature that coincides with the dust tail. To the best of our knowledge, a secondary neutral sodium tail feature of this sort has not been observed at comet Hale-Bopp, but that may be the result of its coincidence with the cometary dust tail. If a similar feature were observed, it may indicate that the source of neutral sodium is within the cometary dust tail.

Near-Sun comets often shown bright orange emission features. Knight et al. [2010a]
suggested that these are likely to be the result of neutral sodium emission. As near-Sun comets typically show very different behaviour to comets like Hale-Bopp, studying the apparent neutral sodium tail features at these objects represented an interesting challenge for COMPASS. In chapter 9 we consider the application of COMPASS to the observations of three near-Sun comets where neutral sodium tails are thought to have been observed. The results of these simulations again show that the correct physical behaviour is reproduced by COMPASS for these very different comets, as the morphology of the neutral sodium tails simulated matches the data. However, the results also show that the $1/r^2$ dust source distribution used in COMPASS is not a good representation of the behaviour of neutral sodium at small heliocentric distances.

Overall, COMPASS has been shown to be well suited to understanding whether a distinct neutral sodium tail feature present in imaging data is consistent with our current understanding of the evolution of neutral sodium in comets. The main achievement of COMPASS is in translating this physics into observational effects that include consideration of the relative motion of the observer and the observational perspective. The model’s success at independently reproducing the observed morphology of neutral sodium tails at a variety of comets is an indication that the evolution of sodium in comets is relatively well represented by the physics of COMPASS and that the initial neutral sodium atom production velocity is possibly similar to that described by COMPASS (i.e. negligible relative to the cometary nucleus velocity). COMPASS is also able to reproduce spectroscopic data, but as these simulations are more sensitive to the initial source distributions the results are not as good a match to the data.

Although the work presented in this thesis is not able to determine the source of neutral sodium in comets, it does represent an important step in the characterisation of the behaviour of neutral sodium at comets and would be well suited to testing additional sodium source distributions in the future.

10.2 Further Work

There are many potential avenues of future research open to COMPASS as its modular design makes it very easy to add new source distributions, parametrisations, observational perspectives and cometary orbits. A more detailed description of the further work following directly from the studies discussed in chapters 6, 7, 8 and 9 are presented in the final pages of those chapters, but some broad themes of further work covering the whole scope of this thesis are discussed in the paragraphs that follow.

**Improving the collisional region parametrisation** The results of chapter 6 strongly suggest that the collision radius should not be modelled as a spherical boundary, as the cometary coma will be slightly compressed in the Sun–comet direction by the solar wind and solar radiation pressure. Modelling the collisional region as a hard,
Further Work

spherical boundary is very computationally efficient but not physically realistic. In reality a much smoother transition from collision-dominated to collision-free regions would be observed, which could be included in COMPASS.

Furthermore the collision radius approximation may not be appropriate when considering observations very close to the nucleus because the relatively dense region of the coma may act as a secondary source of solar radiation via scattering of sunlight (see e.g. Fernandez [1999]). Some authors have speculated that even within the densest parts of the cometary coma, reradiation compensates for the decrease in sunlight (e.g. Salo [1988]) and inclusion of this process may improve the simulation.

An additional loss mechanism? The results of the imaging studies (chapter 7, 8 and 9) show that the simulated neutral sodium tail is too high in intensity far from the comet nucleus. The dominant brightness effect in COMPASS in all these simulations is the loss due to photoionisation, so if additional loss is important it may be prudent to study the effect of including an additional loss parameter of the form:

\[ S \propto e^{-t/\tau} \]  

(10.1)

where \( \tau \) is to be determined. To date photoionisation is considered to be the dominant loss process for cometary sodium, but this may the result of the focus of previous studies close to the comet nucleus. Additional loss processes, such as electron and ion impact ionisation, may also be important at large cometocentric distances. The neutral sodium tail of comet Hale-Bopp persisted well away from the comet, and was in the solar wind downstream of the comet. As the plasma number density is lower in the solar wind downstream of the comet, the loss rate due to electron and ion impact ionisation in the neutral sodium tail of comet Hale-Bopp far from the nucleus is likely to be lower than in the coma. This would have the effect of reducing the intensity of the neutral sodium emission close to the comet nucleus and therefore increasing it (relatively) at larger cometocentric distances, effectively resulting in a longer neutral sodium tail than currently simulated.

For the spectroscopy study (chapter 6) the dominant brightness effects are the decrease of photon intensity with the square of heliocentric distance and the number of particles in the simulation, which is expected as on the small scales considered in this study as a significant time has not passed since production for the COMPASS particles within the slit close to the cometary nucleus. An additional loss process is unlikely to have an effect on simulation results in this region, even if it is present. Studies determining the effect of sublimation of neutral sodium and the characteristic photoionisation lifetime for neutral sodium at very small heliocentric distances may also be useful for simulating near-Sun comets.
Determining more appropriate source distributions  In the first instance a more complex, Monte-Carlo cometary dust tail model could be incorporated in COMPASS to continue the study presented in chapter 8. A study considering the effect of including additional velocities in the source distribution could also be considered.

In the future more data (particularly in situ data obtained at comet 67P/Churyumov-Gerasimenko by the Rosetta spacecraft, see Wurz et al. [2015]) may be available on the source of neutral sodium in comets. It is likely that the source of neutral sodium may be different for comets of different activities (e.g. sputtering will dominate for low activity comets, but other processes may dominant for comets with higher activities), but once the possible sources have been characterised through study of in–situ data or appropriate laboratory work, models like COMPASS will be very effective at determining which processes dominate at which comets, which could ultimately determine whether (if any) neutral sodium is present within cometary ice and therefore indicate whether significant nucleogenic heating was present during the formation of the solar system within the cores of comets (as discussed by Ellinger et al. [2015]).

Studying new sodium tail features  In order to determine whether the effects observed at the comets studied in this thesis are universal, COMPASS should be applied to as many observations of neutral cometary sodium features as possible. In the first instance the model should be applied to additional images of comets with prominent neutral sodium tail features observed by the C2 and C3 coronagraphs on SOHO/LASCO. If additional gravitational effects were included, COMPASS could also be used to simulate the neutral sodium tail observed at Mercury (e.g. Baumgardner et al. [2008]) and the Io torus at Jupiter (e.g. Mendillo et al. [2007]).

Can the neutral sodium production rate be determined using COMPASS? Relative brightness effects were considered in chapters 7 and 8 because calibrated CoCam images of comet Hale-Bopp were unavailable. In chapter 9, relative brightness effects were considered primarily as a result of the processing required to facilitate direct comparison between the LASCO images and the results of COMPASS. However, even if calibrated, processed LASCO images were available in a suitable format it would not be possible to independently estimate the production rate of neutral sodium using COMPASS as it is currently formulated. COMPASS simulations are said to be converged (and therefore representative of the behaviour at the comet) when the change between consecutive simulations is below a chosen threshold. The number of COMPASS particles required to reach convergence depends primarily on the orbit of the comet and the observational perspective that produced the image. Therefore the number of COMPASS particles in the converged simulation is independent of cometary characteristics like activity that determine neutral sodium production rate. If more computational resources were available, it may be possible to use one COMPASS par-
article to represent $n$ neutral sodium atoms, but in this case convergence would not be applicable and the robustness of the result would be difficult to verify except through trial and error using a large number of observations.

However, it would be possible to converge the heliocentric velocities of neutral sodium in a COMPASS simulation, in the manner described in chapter 6. COMPASS is therefore capable of predicting neutral sodium atom velocities given suitable initial source distributions, which could then be used to estimate the neutral sodium production rate at the comet.
Appendices
Appendix A

Comet Orbital Elements, Taxonomy and the Origins of Comets

Comets are typically classified by their orbital elements. Six orbital elements fully describe a given comet’s orbit:

- Perihelion distance, $q$: Comet’s heliocentric distance at perihelion.
- Eccentricity, $e$: Defines whether the orbit is a circle ($e = 0$), ellipse ($0 < e < 1$), parabola ($e = 1$) or hyperbola ($e > 1$)
- Inclination, $i$: Angle between ecliptic and the comet’s orbital plane.
- Argument of perihelion, $\omega$: Angle between the point where the comet crosses the ecliptic (on the portion of its orbit that goes from below the ecliptic to above it) and the perihelion position.
- Longitude of ascending node, $\Omega$: Angle between the point where the comet crosses the ecliptic (on the portion of its orbit that goes from below the ecliptic to above it) and vernal equinox.

If the comet’s orbit is elliptical, it may also be useful to consider the semi-major axis, which is the line that runs from the centre of the ellipse through one focus to the perimeter. Studying the semi-major axis, usually denoted by $a$, gives an insight into the outermost distances reached by the comet during its orbit.

A diagram showing a typically used classification scheme, based on a comet’s orbital elements, is given in figure A.1. Long period comets, with periods of approximately 200 years or greater are considered to have their origins in the Oort cloud. Long period comets are classified as dynamically new if it is assumed to be their first transit to
the inner solar system and are classified as returning comets if this is not the case. Dynamically new comets are usually classified as such if their $1/a$ lies within the peak in this distribution observed for long period comets shown in figure A.2. A dynamically new comet that has travelled into the inner solar system once will gain approximately $\pm 0.005\,\text{AU}$, and as the peak in the $1/a$ distribution for these objects is extremely narrow, this would result in a value of $1/a$ for this object that would no longer lie on the peak. Dynamically new comets may also be identified by particularly strong continuum features in their spectra Oort and Schmidt [1951]. Short period comets are typically classed as Halley-Type comets or Jupiter–family comet. There are new specialised classifications currently in use such as Enke-type, Chiron-type and multiple classifications within groups. See for example Wang and Brasser [2014]; Horner et al. [2003]; Levison [1996] for more discussion on this topic.

It is difficult to classify comets based only on their period and semi major axis, as in this scheme some comets may change from one scheme to the next. Therefore a new scheme, based on the Tisserand parameter with respect to Jupiter, has been proposed. The Tisserand parameter is defined as Duncan et al. [2004]:

$$P_T = a_J/a + 2 \cos(i) \sqrt{(1 - e^2) a/a_J}, \quad (A.1)$$

where $a_J$ is Jupiter’s semi major axis, $a$ is the comet’s semi major axis, $e$ is the comet’s eccentricity and $i$ is the comet’s inclination. The Tisserand parameter defined in this way gives an indication of the relative velocity, $v_{rel}$, between Jupiter and the comet during a close encounter using the equation Duncan et al. [2004]:

Figure A.1: Diagram indicating the typical classifications of a comet, based on orbital characteristics. $P$ is the period of the comet’s orbit and $a$ is its semi-major axis. Reproduced from Levison [1996].
Figure A.2: Distribution of semi-major axes of observed long period comets. $a$ is the semi-major axis of the comet’s orbit and $1/a$ is proportional to the orbital binding energy. Reproduced from Levison [1996], from data presented in Marsden and Williams [1992].

$$v_{rel} = v_c \sqrt{3 - P_T} ,$$  \hspace{1cm} (A.2)

where $v_c$ is Jupiter’s velocity with respect to the Sun. Therefore objects with $P_T < 3$ have very slow relative velocities with respect to Jupiter during close encounters and consequently can be greatly affected by its gravitational field. Objects in circular orbits with $P_T > 3$ would be confined either within the orbit of Jupiter or externally to Jupiter’s orbit, as they have very little interaction with Jupiter’s gravitational field.

A classification based on the Tisserand parameter allows the source of groups of comets to be more easily identified. This classification was presented in Duncan et al. [2004]. Comets with $P_T > 2$ (e.g. Jupiter–family comets typically have $2 < P_T < 3$) are described as ecliptic comets, because most members of this group have small inclinations relative to the ecliptic. Therefore the most likely source of these objects is the Kuiper Belt and Scattered Disk. Comets with $P_T < 2$ are likely to have a range of inclinations, and therefore are described as nearly isotropic and most probably originate in the Oort cloud.
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