

Chapter 4

Coma

Volatile components of the nucleus are sublimated by solar radiation. When leaving the surface the gas picks up dust particles and drags them outward. Gas and dust together form the coma around the nucleus. The activity of a comet depends on two factors: its composition and its distance from the Sun. The activity increases with diminishing distance from the Sun.

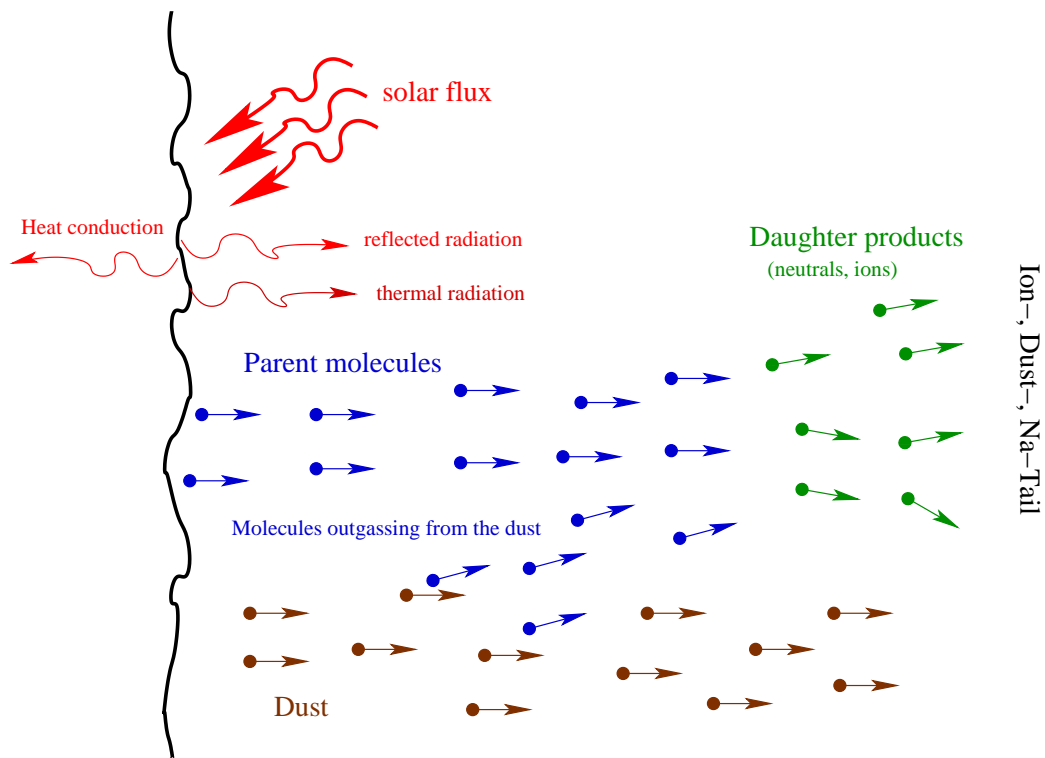


Figure 4.1: A schematic view of the process leading to the formation of the coma and the tail, as well as the main processes within the coma (Drawing based on [Rauer, pers. comm.])

Figure 4.1 is a very simplified view of the processes leading to the formation of the cometary

coma and of the processes within the coma. The coma has two main constituents, the gas coma (blue and green in figure 4.1) and the dust coma (brown in figure 4.1). The gas coma consists of molecules sublimated from the nucleus by solar heating. Once leaving the nucleus, molecules in the coma are exposed to direct solar radiation and can react in various ways. Ultimately most molecules are dissociated or ionized within a day after leaving the nucleus surface (see dynamics below). By convention, the initial molecule is often referred to as the "parent molecule" (blue in figure 4.1) while the fragments produced during the dissociation processes are known as "daughter" molecules or radicals (green in figure 4.1).

The daughter molecules are quite easily observable in the optical wavelengths range. CN, C₂, C₃ and NH₂ have strong emission lines which can be easily detected in most comets. This is the reason why these molecules have received so much attention in cometary research. However they are only a tracer for the parent molecules which are much more difficult to observe. The direct study of parent molecules is possible only in the infrared or submillimeter wavelength range.

The dust coma (brown in figure 4.1) consists of dust grains dragged from the nucleus by the sublimating gas. At a distance from the nucleus equivalent to a few tens of the nuclear diameter the dust grains effectively leave the gravitational field of the nucleus. They are on their own orbit around the Sun. The speed of the dust grains depends on their size. Very small grains are quickly accelerated to the gas speed, while larger grains may be too heavy to reach more than a fraction of the gas speed. Only grains with a terminal speed greater than the escape velocity of the nucleus can be ejected. The larger grains will ultimately fall back to the nucleus surface and can possibly form a dust mantle. For a more detailed discussion of the cometary dust coma see for example Knollenberg [1993] and, especially for the dust coma of comet Hale-Bopp Weiler [2002]. The dust coma itself can contribute to the gas coma, under the assumption that the dust grains contain volatiles. These can sublimate and the dust grains become a so-called 'extended source' for the gas.

Dynamics

The outflow speed of the coma is comparable to the speed of sound in the coma gas at the temperature of the nucleus. For a comet near the orbit of the Earth, this is about 1 km/s. This speed and the lifetime of molecules against photo destruction together determine the scale of the cometary coma. Assuming typical lifetimes of molecules in the coma, at 1 km/s, these molecules can travel about 90,000 km and this is the approximate radius of the gas coma (approx. 10^5 km).

Close to the nucleus the density is high enough for frequent collisions. In this region the coma dynamics can be described by the laws of classical hydrodynamics. The density in the coma decreases rapidly with nucleocentric distance and the gas flow transits to a free molecular flow.

The flow can be described as a supersonic jet. The result is an adiabatic expansion, in which no energy is exchanged with the environment. The pressure, build up by sublimation on the cometary surface, is transferred continuously to the nearly vacuum conditions of the

interplanetary space. The expansion is accompanied by a sudden and significant drop in the temperature, combined with an acceleration of the gas. However the assumption of an ideal adiabatic expansion is not valid for the real conditions in a cometary coma. For a more realistic discussion of the dynamics see section 12.1 on page 105.

Interaction with solar pressure

Solar photons can have an effect on the dynamics of molecules in the coma. The absorption and re-emission of solar photons induce a force on each particle known as radiation pressure. With the emission rate or g factor as it will be defined in section 5.2 the acceleration a of a particle due to this effect is

$$a = \frac{h}{m} \sum_i \frac{g}{\lambda_i} \quad (4.1)$$

where h is the Planck constant and m is the molecular mass. Using this equation the acceleration a can be calculated for some of the smaller molecules which are most affected.

Species	a [cm s ⁻²]
H	0.8
CN	0.27
C ₂	0.22

Table 4.1: Acceleration due to solar wind pressure

The acceleration varies with the solar flux as r_h^{-2} . The radial component of the velocity of the molecules is reduced to zero on the sunward side of the coma in the time v/a where v is the velocity of the molecules after leaving the surface. The distance

$$d_s = \frac{v^2}{2a} \quad (4.2)$$

at which the outward motion of the molecules stall is called the 'stand-off' distance. For C₂ at $r_h = 3$ AU with a velocity of $v = 0.7$ km/s the stand-off distance d_s is approximately $6 \cdot 10^6$ km. Thus the effect is negligible at larger heliocentric distances. However closer to the Sun it has to be taken into account when studying the spatial structure of the coma.

Chemistry

The chemistry in a cometary coma is rather complex. This section will only give a very brief overview. For more details see the section 12 on the Comchem model. The analysis of the complex formation chemistry of C₂ and C₃ is the main tasks of this work, see section V on page 93.

Table 4.2 gives an overview of the different types of reaction in a cometary coma. The table is based on the reaction network by Schmidt *et al.* [1988] and Huebner *et al.* [1987] as

it is implemented in the ComChem model (see section 12). The size of the collision zone is determined by the activity of the comet. The sizes of the comet collision zone and the ionopause scale roughly with the water production rates (Wegmann [1995] and especially for Hale-Bopp Flammer *et al.* [1997]). While it is typically around $\rho_{\text{coll}} \sim 10^3$ km nucleocentric distance for moderately active comets it was as large as $\rho_{\text{coll}} \sim 10^5$ km for comet Hale-Bopp at its perihelion (derived from Wyckoff *et al.* [1999]).

At the heliocentric distance range $r_h > 2.8$ AU, mainly studied in this work, most of the coma is dominated by photolytic reactions and electron impact reactions. Therefore only these two reaction categories will be discussed in more details in the following two sections. However, it is important to keep in mind, that the relative importance of the reaction categories can change at smaller heliocentric distances.

Photodissoziation	$\text{C}_2\text{H}_2 + h\nu$	\rightarrow	$\text{C}_2 + \text{H}_2$
Photoionization	$h\nu + \text{C}_2\text{H}_2$	\rightarrow	$\text{C}_2\text{H}_2^+ + e$
Photodissociative ionization	$\text{CO}_2 + h\nu$	\rightarrow	$\text{O} + \text{CO}^+ + e$
Electron impact dissociation	$\text{C}_2\text{H}_2 + e$	\rightarrow	$\text{C}_2 + \text{H}_2$
Electron dissociative recombination	$\text{C}_2\text{H}^+ + e$	\rightarrow	$\text{C}_2 + \text{H}$
Electron impact electronic state excitation	$\text{CO}(^1\Sigma) + e$	\rightarrow	$\text{CO}(^1\Pi) + e$
Electron impact ionization	$e + \text{CO}$	\rightarrow	$\text{CO}^+ + 2e$
Electron impact dissociative ionization	$e + \text{CO}_2$	\rightarrow	$\text{O} + \text{CO}^+ + e$
Positive ion charge transfer	$\text{H}_2^+ + \text{C}_2\text{H}_2$	\rightarrow	$\text{C}_2\text{H}_2^+ + \text{H}_2$
Positive ion-atom interchange	$\text{H}_2^+ + \text{C}_2\text{H}_2$	\rightarrow	$\text{C}_2\text{H}_3^+ + \text{H}$
3-Body positive-neutral association	$\text{C}_2\text{H}_2^+ + \text{H}_2 + \text{M}$	\rightarrow	$\text{C}_2\text{H}_4^+ + \text{M}$
3-Body neutral recombination	$\text{C}_2\text{H}_2 + \text{H} + \text{M}$	\rightarrow	$\text{C}_2\text{H}_3 + \text{M}$
Hydrogen impact dissociation	$\text{CH}_4 + \text{H}$	\rightarrow	$\text{CH}_3 + \text{H} + \text{H}$
Radiation stabilized neutral recombination	$\text{C} + \text{C}$	\rightarrow	$\text{C}_2 + h\nu$
Radiation stabilized positive ion-neutral association	$\text{C}^+ + \text{H}$	\rightarrow	$\text{CH}^+ + h\nu$
Radiative electronic state deexcitation	$\text{O}(^1\text{D})$	\rightarrow	$\text{O}(^3\text{P}) + h\nu$
Neutral rearrangement	$\text{N} + \text{CH}$	\rightarrow	$\text{CN} + \text{H}$
Neutral impact electronic state quenching	$\text{O}(^1\text{D}) + \text{CO}_2$	\rightarrow	$\text{O}(^3\text{P}) + \text{CO}_2 + h\nu$
Neutral-neutral associative ionization	$\text{CH} + \text{O}$	\rightarrow	$\text{HCO}^+ + e$
Radiative recombination	$e + \text{C}^+$	\rightarrow	$\text{C} + h\nu$

Table 4.2: Overview of the gas-phase reaction categories in a cometary coma with examples (adapted from Schmidt *et al.* [1988])

Photolytic reactions

Dissociation or ionization by solar photons are the most dominant processes in a cometary coma. The coma itself is in general optically thin except for the proximity of the nucleus. Here the lines of some species such as water can become optically thick, especially for the ultraviolet continuum beyond the dissociation limit for H_2O . Only for very dusty comets the innermost coma ($\rho \sim 100$ km) may be optically thick even in the optical wavelength range. It is thus valid to assume that for most of the coma each molecule or radical is irradiated with

sunlight. Each molecule has a lifetime versus dissociation or ionization that varies with the solar flux as r_h^{-2} . The reciprocal of the lifetime, the rate coefficient k for photodissociation or -ionization is obtained easily by the following relation

$$k = r_h^{-2} \cdot \int_0^{\lambda_0} \sigma(\lambda) F_{\odot}(\lambda) d\lambda \quad (4.3)$$

r_h	heliocentric distance [AU]
$\sigma(\lambda)$	cross section for dissociation or ionization
$F_{\odot}(\lambda)$	solar flux
λ_0	threshold wavelength for dissociation or ionization

One of the most complete lists of reaction coefficients is given by Huebner *et al.* [1992]. For a comparison of lifetimes against photodissociation of some of the important species for the cometary coma determined by various authors see Crovisier [1994] and reference therein. The simplicity of equation (4.3) suggested, that the reaction rate coefficients are readily available. However this is not the case, because for many species the cross section $\sigma(\lambda)$ is not well known over large parts of the spectrum. The situation is complicated further by the branching ratio among various reaction pathways. Last but not least the solar spectrum $F_{\odot}(\lambda)$ is not constant. Apart from short term variation it shows a long term variation with the solar cycle. The dissociation of H_2O can serve as an example for the discussed complications. This table is taken from Huebner *et al.* [1992]. While the first reaction coefficient was calculated for the case of quiet Sun, the second is for the active Sun.

Reaction	k	k
$\text{H}_2\text{O} + h\nu \longrightarrow \text{OH} + \text{H}$	$1.03 \cdot 10^{-5} \text{s}$	$1.76 \cdot 10^{-5} \text{s}$
$\longrightarrow \text{H}_2 + \text{O}(^1\text{D})$	$5.97 \cdot 10^{-7} \text{s}$	$1.48 \cdot 10^{-6} \text{s}$
$\longrightarrow \text{H} + \text{H} + \text{O}$	$7.55 \cdot 10^{-7} \text{s}$	$1.91 \cdot 10^{-6} \text{s}$
$\longrightarrow \text{H}_2\text{O}^+ + \text{e}$	$3.31 \cdot 10^{-7} \text{s}$	$8.28 \cdot 10^{-7} \text{s}$
$\longrightarrow \text{H} + \text{OH}^+ + \text{e}$	$5.54 \cdot 10^{-8} \text{s}$	$1.51 \cdot 10^{-7} \text{s}$
$\longrightarrow \text{H}_2 + \text{O}^+ + \text{e}$	$5.85 \cdot 10^{-9} \text{s}$	$2.21 \cdot 10^{-8} \text{s}$
$\longrightarrow \text{OH} + \text{H}^+ + \text{e}$	$1.31 \cdot 10^{-8} \text{s}$	$4.07 \cdot 10^{-8} \text{s}$

Table 4.3: Reaction coefficients k for dissociation of H_2O [Huebner *et al.*, 1992]

In nearly all of these reactions the fragments receive an excess energy, which basically leads to an acceleration of the lightest fragment. This has to be taken into account for a proper modeling of the chemistry and dynamics.

Electro impact dissociation

The example of the photolytic destruction of water shows, that a number of electrons can be produced as a byproduct. Apart from water there are further molecules producing electrons

by ionization reactions (see section 12). Another source for electrons in the coma is the solar wind. If the kinetic energy of these electrons is high enough, in other words if they are hot enough, they can destroy further molecules by electron impact dissociation or ionization. The reaction coefficient k can be described in the standard Arrhenius form

$$k = A \left(\frac{T_e}{300} \right)^B \exp -\frac{C}{T_e} \quad (4.4)$$

T_e electron temperature
 A, B, C Arrhenius coefficients

The dependence on heliocentric distance is now folded into the electron temperature T_e . The problem of the unknown cross section, converted to Arrhenius coefficients A, B, C , is for electron impact dissociation even more severe than for photodissociation. Only recently some work has been start and first cross sections are now available (see for example Pang *et al.* [1987] on methane and acetylene and Alman and Ruzic [2000] for a general study on hydrocarbons).