Oxygen-rich AGB stars with low mass-loss rate observed with Herschel

Chousinho Khouri Silva, T.

Citation for published version (APA):
The asymptotic giant branch (AGB) is a phase in the lives of low- and intermediate-mass stars (0.8 – 8 $M_\odot$) when intense ($10^{-8} – 10^{-4}$ $M_\odot$ year$^{-1}$), slow ($\sim 10$ km s$^{-1}$) winds occur. The conditions for the development of these outflows are met because of the low effective temperatures, large amplitude pulsations, and high luminosities all characteristic of the AGB phase. The composition of the material ejected into the interstellar medium during the AGB phase differs from the initial composition of the star because it contains elements that were synthesized in the stellar core and brought to the surface by convective streams. This makes AGB stars important players in the chemical evolution of galaxies. Moreover, the mass-loss is so strong that it becomes the main process regulating the evolution of these stars from the beginning of the AGB.

The mass-loss is understood as a two-step process which requires the enlarged density scale-heights produced by pulsations and the subsequent formation of dust grains. Once solid particles form, the continuum opacity provided by them absorbs momentum from the radiation field. Due to the high densities in the region where the outflow is initiated, the momentum acquired by the dust grains is quickly shared with the gas through collisions. Because of the high luminosities of the stars there is enough momentum in the radiation fields to drive the outflows.

Despite our good qualitative understand of how the AGB winds come about, predicting the mass-loss of an AGB stars from first principles in not yet possible. This is because of the complexity of the region from where the winds are launched and the difficulties in modelling the formation and growth of solid particles in this environment. This complexity makes theoretical prediction difficult, and it is therefore important to characterize these winds from an observational perspective in order to advance our understanding of the AGB phase. This is also not an easy task, since
important parameters such as the stellar mass and the evolution of the mass-loss rate in time are difficult to determine for a given AGB star.

This thesis is a step in the direction of a deeper understanding of the mass-loss in AGB stars. Its main subject is a subset of the AGB population, low mass-loss rate, oxygen-rich AGB stars. We study these sources by combining and modelling different datasets. In particular, we use exceptional data obtained with the Herschel observatory and analyze the data using state-of-the-art radiative transfer codes for the dust component (MCMax) and molecular gas (GASTRoNOoM) together and in a consistent way. In this introductory chapter, we present the current knowledge of AGB stars and their mass-loss process to contextualize the findings presented and discussed in the following chapters. Most of the text of this introduction is based on the books “Asymptotic giant branch stars” edited by Habing & Olofsson (2003), “Astro-mineralogy” edited by Henning (2010), “Introduction to stellar winds” by Lamers & Cassinelli (1999), and “Stellar structure and evolution” by Kippenhahn et al. (2012). The reader is referred to those when no reference is given.

1.1 History

The existence of very luminous stars, that were soon termed “giants”, was known since the beginning of the 20th century (Hertzsprung 1905) but until the 1950’s the evolutionary stage of these stars remained unclear. After the discovery of the hydrogen burning processes, the pp-reaction and the CNO-cycle, that provide energy to stars during the main sequence (Bethe 1939), models that reproduced and explained the stellar structure in this phase quickly developed. However, it was only in 1952 that Sandage & Schwarzschild produced the first virtual red giant stars from considering models with hydrogen-exhausted cores, which undergo gravitational contraction and release energy. A few years later, the evolution of low- and intermediate-mass stars until the horizontal branch was already understood. The understanding of the AGB phase, first identified as a “bifurcation of the giant branch”, and the discovery of the mass-loss from these objects happened in the subsequent decades, as theoretical comprehension and observational techniques developed.

The 1960’s were important years for the research of cool giants. During this decade infrared observations of astronomical sources developed and the first circumstellar molecular line was detected at radio wavelengths due to maser emission of OH in the circumstellar environment of a supergiant star (Wilson & Barrett 1968). The new observations and other evidence suggested that AGB stars lose mass in a dense outflow, a picture that with time became widely accepted. The infrared windows for ground-based observations allowed astronomers to discover large infrared excess in red giants, which was attributed to the presence of circumstellar dust. Sil-
icantes were the first dust species identified around oxygen-rich AGB stars in 1968 (Gillet et al. 1968). Soon the dichotomy between carbon-rich and oxygen-rich AGB stars, that was known from molecular absorption bands for more than one century and explained in terms of the high binding energy of CO (Russell 1934), was also observed in the infrared excess (Woolf & Ney 1969). Theory also advanced quickly in the 1960’s. For instance, thermal pulses (named He-shell flashes at first), a process that happens during the AGB due to instabilities in the burning layers, were serendipitously discovered from evolutionary calculations by Schwarzschild & Härm (1965). Schwarzschild & Härm (1967) showed that the thermal pulses could be responsible for bringing processed material from the stellar interior to the surface, changing the composition of the outermost layers. More accurate calculations of thermal pulses became possible with increasing computer power and these models reached higher levels of details in the 1970’s. Another important insight came in 1966, when Wickramasinghe et al. revealed a mechanism for mass loss in red giants. The authors proposed that radiation pressure acting on dust grains would be able to drive a wind. This is the mechanism still widely accepted to this day.

In the 1970’s, the first line from a thermally excited transition (CO $\nu = 0, J = 1 - 0$) was detected (Solomon et al. 1971) in IRC+10216. With the construction of a large number of radio-telescopes in the following years, the number of sources and molecules detected rapidly multiplied. The study of CO emission lines remains the most widely used method for determining the mass-loss rates and expansion velocities of AGB stars. The increasing amount of information on AGB stars led to the development of a spherical model of the envelopes around OH/IR stars (strongly obscured AGB stars that present OH maser emission) by Goldreich & Scoville in 1976. The model brought together the knowledge on AGB winds, made predictions of very high mass-loss rates, and explained how the maser emission was produced. In 1975, Iben was also able to explain the formation of carbon stars due to the thermal pulses.

With the structure and evolution of AGB stars well understood, the next revolution came with the launching of the infrared astronomical satellite (IRAS) in 1983. IRAS performed an unbiased scan of the infrared sky and detected hundreds of thousands of sources. From its data with unprecedented spectral coverage and resolution in the near-infrared, a new era of statistical analysis of a large number of AGB stars with dust envelopes started. From then on, observations from the ground benefited immensely from the invention of new techniques and the construction of increasingly better instruments.

The story of the following decades in AGB research consists of insights that led to the discovery of many unexpected new aspects of AGB stars and of deeper understanding of the mechanisms behind the observed properties of these objects. This research has essentially confirmed and refined the framework that had been achieved
1 Introduction

by the beginning of the 80’s, and which was crowned by the seminal review of Iben & Renzini (1983). Nonetheless, despite the fact that the overall picture we have of AGB stars seems to be correct and that our understanding of it is improving progressively, many questions still remain open in the field. In the following pages we will delve into some of those.

1.2 Evolution up to the AGB

Stars form from gas in molecular clouds, which can have up to millions of solar masses. When perturbations in the structure of a given cloud (e.g. due to shocks or tidal forces) make the cloud (or a part of it) unstable against its own gravitational pull, a gravitational collapse is triggered. That happens in a hierarchical manner as instabilities propagate to smaller scales. From the cores that have masses of the order of the final stellar masses, a star (or stars) and planetary systems are born. These stellar-mass blobs of gas continue to collapse under the influence of their own gravity, heating its denser core. When the temperature becomes high enough in the centre, thermonuclear burning sets in. It can be said that the tale of the lives of low- and intermediate-mass stars is the struggle between the gravitational pull and
the counterbalance due to pressure from the particles that constitute them. Energy produced by nuclear burning continuously replenishes what is lost by radiation and allows stars to remain in stable configurations for long periods of time. As these stars evolve they undergo many different processes that are triggered mainly by the exhaustion of fuel. Those changes are reflected in observables such as temperature and luminosity and the evolution of stars can be followed in the Hertzsprung-Russell diagram, as shown in Fig. 1.1.

Stars start their lives on the zero-age main-sequence (ZAMS) with the onset of hydrogen burning in the core, where temperature and pressure are high enough. They spend about 90% of their lives in this configuration. The mechanism of hydrogen burning depends on the initial stellar mass and changes progressively from lower mass star with $M \approx 0.8 \, M_\odot$ to higher mass stars with $M \geq 2 \, M_\odot$. For stars with masses about that of the Sun, the proton-proton (pp) chain dominates the energy production on the main sequence. For stars more massive than about $2 \, M_\odot$, the CNO-cycle is responsible for most of the energy produced. The production of energy via the CNO-cycle depends much more strongly on temperature than the pp-chain does. Because of this, as the temperature in the core increases, for stars with progressively higher masses, the CNO-cycle gradually takes over as the main energy production mechanism. Since there is no process that keeps the stellar material well-mixed (except for very-low mass stars, $M \leq 0.5 \, M_\odot$), stars develop a heterogenous structure. Hydrogen is progressively consumed in the core but its abundance remains virtually unchanged in the outer stellar layers.

When about 10% of the total hydrogen content of low- and intermediate-mass stars is consumed, the core has become helium-rich and mostly hydrogen-free. Burning of hydrogen shifts from the centre to the inner-most hydrogen-rich shell. Because of the low energy production rate in the centre, the core contracts. The gravitational energy released by the helium-rich core stimulates hydrogen burning and energy production in the hydrogen-burning layer. An important detail is that the equilibrium temperature of the high-mean-molecular-weight gas in the helium core is higher than for hydrogen-rich gas. Because of the strong temperature dependence of hydrogen burning through the CNO-cycle, the heated hydrogen-burning shell produces more energy than can be transported outwards, even by convection. The only solution is for these stars to experience a large expansion. As more helium is deposited in the core from the burning of hydrogen, the temperature increases at the hydrogen-burning layer and, hence, the energy production. This leads to further expansion and increase in luminosity. A small increase in the helium core mass causes a sizable envelope expansion and the stars expand quickly and become luminous, cool giants. The hydrogen envelope turns completely convective. At the beginning of the red giant branch (RGB) phase, the convective envelope penetrates deep enough and reaches
into regions where the chemical composition has been modified by nuclear burning. This leads to a surface enrichment and is referred to as the first dredge-up (see Fig. 1.1). The changes in surface composition due to the first dredge-up are mainly related to the elements involved in the CNO-cycle: carbon, nitrogen, oxygen, and their isotopes. The effect of the changes in the surface isotopic ratios is seen from observations and confirms the occurrence of both the CNO-cycle and the first dredge-up. Moreover, some of these changes are very sensitive to stellar parameters and can be used to constrain them. In particular, the values of the surface isotopic ratios \(^{13}\text{C}/^{12}\text{C}\) and, especially, \(^{17}\text{O}/^{16}\text{O}\) (Boothroyd et al. 1994) after the first dredge-up depend on the initial stellar mass and might be used to determine this elusive parameter of AGB stars. We apply this diagnostic to constrain the mass of W Hydreae in Chapter 2. The stars remain in the RGB phase until helium is ignited in the core.

The ignition of helium can happen either explosively or quiescently, depending on whether the helium core becomes electron degenerate or not before the core ignites. Degeneracy develops if the temperature is not high enough for all electrons in a given volume to occupy different quantum states. For stars with less than about 2.25 \(M_\odot\) the core is so compact compared to the temperature it reaches that electron degeneracy sets in. In degenerate matter, quantum degeneracy – which is independent of temperature – provides most of the pressure. The helium nuclei do not become degenerate, however, and continue to have speeds described by the Maxwell velocity distribution even in a electron degenerate environments. As the core grows, the temperature of the non-degenerate particles increases until the temperature for the occurrence of the triple-\(\alpha\) (helium burning) reaction is reached. When that happens, the energy produced by nucleosynthesis does not lead to an expansion of the nucleus and a run-away burning situation develops. Higher burning rates lead to higher temperatures that lead to even higher burning rates. For a few seconds, the luminosity produced is comparable to that of an entire galaxy. But most of the energy never makes it to the surface, as it is used to lift the degeneracy from the nucleus and to expand of the core. The stars which do not reach the conditions for electron degeneracy in the core ignite helium in a non-explosive way when the temperature is high enough. At this point, the stellar structure consists of a helium-burning core and a hydrogen-burning shell. The star will remain in this stable configuration for a time that is equivalent to about 10% of the main-sequence time.

After burning most of the helium in the core similar conditions to the one encountered at the end of the main sequence are reached. The helium-depleted core is now carbon- and oxygen-rich. The energy production in the centre decreases as the helium atoms become rarer and helium burning shifts to the innermost helium-rich shell. As for the first ascent on the red giant branch, the luminosities produced by the helium- and hydrogen-burning layers reflect what happens in the core. Again, the
1.3 Evolution on the AGB

On the early-AGB, the stellar structure is basically independent of stellar mass and consists of helium- and hydrogen-burning shells and an inert, electron degenerate carbon and oxygen core (see Fig. 1.2). Further nuclear burning of carbon into heavier elements does not occur for stars with masses larger than \( \sim 8 \, M_\odot \), setting an upper limit to the mass of AGB stars. Initially, helium burning dominates the energy output on the AGB but as the evolution proceeds, the helium shell becomes thinner and the temperature and energy production in the hydrogen burning shell rise. Eventually, the energy production from hydrogen burning becomes the main contributor to the stellar luminosity. The helium shell continues to become thinner, since helium burning happens faster and produces less energy than hydrogen burning, and when an optimal shell thickness is reached an important process named thermal pulse arises (Schwarzschild & Härm 1965) and the star enters the thermally pulsing AGB.
AGB) phase (see Fig. 1.1).

A thermal pulse happens if the helium shell is thin enough for an expansion to lead to a small decrease in the shell pressure and thick enough for energy produced in the shell not to be lost easily to neighbouring shells. If those conditions are fulfilled, a positive temperature perturbation in the shell will lead to a runaway situation. Because an increase in the temperature of the shell increases the energy production and causes an expansion and a drop in the density of the shell. If this expansion does not reduce the pressure from the upper layers by a factor equal or greater than that of the density decrement, the temperature will rise instead of declining. A higher temperature, then, leads to higher energy production, which causes the temperature to rise in a runaway process. The cycle is broken when the helium shell has greatly expanded and most of the fuel has been used. The expansion is so large that the hydrogen burning stops momentarily and the convective region in the envelope becomes less deep (see Fig. 1.3). Once the helium shell contracts again, hydrogen burning resumes. Helium continues to be produced until the helium shell reaches the required conditions for a new thermal pulse to occur, and the process repeats itself. The time between two pulses is of the order of $10^5$ years (but can be as low as $\sim 10^4$ years for the more massive AGB stars, with $M \sim 5 M_\odot$) and helium-shell burning happens only for a few hundred years.

A very high luminosity is produced in the helium-burning shell during a thermal pulse but most of the energy is used in the expansion of the upper layers. The very high energy production causes convection zones to develop and that leads to the dredge-up of processed material. This is referred to as the third dredge-up (see Fig. 1.3) and consists of a collection of individual events that follow each thermal pulse. The third dredge-up has strong effects on the surface composition of AGB stars.

1.3.1 The third dredge-up

A pulse-driven convective zone (PDCZ) is created by the onset of burning in the helium-shell between the helium- and hydrogen-burning shells. The convective streams last for a few hundred years and the composition in this region is homogenized, consisting mainly of helium (75%) and carbon (22%). As shown in Fig. 1.3, when the helium burning ceases and hydrogen burning resumes, the convective streams from the envelope extend deeper and reach the region in which the composition was modified by the PDCZ. This matter with altered elemental composition is mixed to the surface material, changing the surface abundances. However, for stars with solar composition and $M \lesssim 2 M_\odot$, the third dredge-up does not take place. For stars with lower metallicity, the mass limit for the third dredge-up decreases (Karakas 2010).

The composition of the matter mixed to the surface depends strongly on the stellar mass and evolutionary stage on the AGB but consists mainly of elements associated...
with H and He burning and those produced by slow capture of neutrons $^1$. One of the most important consequences of the third dredge-up is the formation of carbon stars (Iben 1975), when the abundance of this element surpasses that of oxygen at the surface. The carbon-to-oxygen ratio is important because it defines the chemistry of the atmosphere and of the circumstellar envelope as a consequence of the high stability of the CO molecule. Since CO can survive at relatively high temperatures and is difficult to dissociate once formed, carbon and oxygen atoms are mostly locked in CO molecules. The remaining oxygen after the formation of CO develops an oxygen-based chemistry, if the abundance of oxygen is higher than that of carbon, while if carbon is more abundant, the chemistry becomes carbon-based. AGB stars that have a C/O ratio close to unity are named S-type stars and present a peculiar chemistry

$^1$Slow refers to the rate at which the neutron capture happens compared to the rate of radioactive $\beta^{-}$ decay. When the neutron flux is low enough for the nucleons to go through a $\beta^{-}$ decay before interacting with the next neutron, the process is said to be slow. If the neutron flux is higher and a given nucleon reacts with more than one neutron before going through a $\beta^{-}$ decay, the process is said to be rapid. Due to the differences in the processes, slow- and rapid-neutron capture produce different elements.
which is not strongly dominated by carbon nor oxygen. The atmospheres of these stars are also polluted by elements produced by slow-neutron-capture nucleosynthesis. For the number abundance of carbon to exceed that of oxygen, large amounts of carbon have to be dragged to the surface. This happens efficient during the third dredge-up in stars with initial masses up to about 4 \( M_\odot \) (e.g. Karaka 2010). For stars with higher masses, hydrogen burning occurs at the base of the convective envelope and the dredged-up material is reprocessed before reaching the surface. Since the burning happens via the CNO-cycle, most of the carbon and oxygen atoms are converted to \(^{14}\text{N}\), and the surface abundance of this element increases substantially. This process is referred to as hot bottom burning and can prevent the formation of carbon stars.

AGB stars are also sites where unique nucleosynthesis happens since matter at the base of the convective envelopes is recurrently exposed to a low flux of neutrons during the TP-AGB, which leads to the production of heavy elements formed only under these conditions. The elements produced via the s-process are observed in the atmospheres of AGB stars confirming its occurrence in the stellar interiors. Some of the elements produced in this way have very short half-lives, such as \(^{99}\text{Tc}\) (having a half-life of \(2 \times 10^5\) years), and are direct evidence of ongoing s-process nucleosynthesis.

1.4 Evolution after the AGB

Evolution on the AGB is terminated when the mass-loss has reduced the hydrogen envelope to \( \sim 10^{-3} M_\odot \). Hydrogen burning still takes place in a shell surrounding the core and the luminosity remains basically unchanged. The effective temperature increases as the hydrogen envelope mass decreases in a well-defined relation (e.g. Schoenberner 1981). If the time is right between the last strong mass-loss rate event and the rise in temperature of the naked core, the system will be seen as a planetary nebulae (Kwok et al. 1978). After hydrogen burning ceases, the remaining carbon and oxygen white dwarf (of typically 0.6 \( M_\odot \)) experiences a slow radiatively cooling.

1.5 The circumstellar envelopes

Despite the effect that processes in the interior of the star have on its structure and chemical composition, it is the characteristic high mass-loss rate (ranging from \(10^{-8}\) up to \(10^{-4} M_\odot\) year\(^{-1}\)) that sets the time-scale of evolution on the AGB. The rate at which AGB stars shed their envelopes is faster than that at which nuclear burning consumes the available fuel. The high mass-loss rates also prevent these stars from ending their lives as supernovas, as stars with masses above \( \sim 1.5 M_\odot \) would explode.
once the fuel was exhausted if no mass loss took place.

The intense mass loss produces a circumstellar envelope that contains several molecules in the gas-phase and different dust species. A schematic view of the structure of a mass-losing AGB star is shown in Fig. 1.4.

### 1.5.1 The mass-loss

The mechanism responsible for mass loss of low- and intermediate-mass stars on the AGB still is the subject of intense investigation. The explanation accepted today was achieved almost half a century ago and relies on the combination of the high luminosities of AGB stars with the continuum opacity provided by dust grains. Although other means of driving the wind of AGB stars (e.g. the combination of pulsation with inefficient radiative cooling, radiation pressure on molecules, and small-scale magneto-acoustic waves) might play a role (Woitke 2003), in this work we focus on the widely accepted picture of dust-driven winds.

For the accepted mechanism to take place, dust grains need to be present in the upper atmosphere. The formation of dust is facilitated by pulsations, which push...
matter away from the star to regions cool enough \((T \leq 1500 \text{ K})\). In this way, the wind of AGB stars is seen as a two-step process that requires pulsations and dust formation to develop.

**Variability and pulsations**

The radial pulsations of AGB stars are observed mainly as photometric variations. The variations in visual magnitude can be 6 mag or more but the bolometric magnitude changes only by \(\sim 1\) mag. The larger variation in flux at short wavelengths is mainly because of two causes: the strong dependence on temperature of the flux of a black-body in this spectral range, for the typical temperatures of AGB stars \((T \sim 2500 \text{ K})\); and the large difference in molecular content of the atmosphere between maxima and minima, which leads to different amounts of absorption of visible radiation. Typical periods range from about a hundred to a few thousand days. From their light curves, these variable stars are morphologically classified in three broad classes: Mira variables, which have large amplitude variations \((> 2.5 \text{ mag in } V)\) and show relatively regular variations; semi-regular variables, that show small amplitude variations \((< 2.5 \text{ mag in } V)\) and less but still definable periodicity; and irregular variables, which show very little periodicity. The last class might be overpopulated by stars with poorly studied light curves. A class of AGB stars that is not represented in this classification scheme are very-high mass-loss rate objects which become completely enshrouded by dust and, hence, too faint in visible light to be detected. These stars are seen to pulsate in the \(K\) band with amplitudes of up to 3 mag and with periods of \(\geq 600\) days (e.g. Le Bertre 1993; Whitelock et al. 1994).

The pulsations create sound waves that propagate through the atmosphere. Because of the characteristic strong radial density gradient that exists in atmospheres, these sound waves develop into shocks. The shocks not only levitate the gas but also heat and compress it, triggering the formation and destruction of molecules and dust. The shocks also contribute to accelerate matter outwards but this push is not enough to overcome the gravitational pull (Höfner et al. 2003). The wind is initiated only if enough dust grains form from the levitated material and provide the opacity for radiation pressure to act transferring the required additional momentum. The gas particles can have a non-negligible contribution to the wind driving by also offering opacity but they are thought to be mainly dragged along by the dust particles via collisions (Gilman 1972). In this sense, dust and gas components of the wind can have different expansion velocities with the dust particles streaming through the gas with drift speeds even higher than the maximum gas expansion velocity.

In the atmospheres of carbon stars the picture of a pulsation-induced dust-driven wind is easy to reproduce, as the most abundant dust species (amorphous carbon) forms very close to the star and provides enough absorption opacity to drive the
The formation and growth of dust grains and the wind driving

The connection between wind driving and grain formation is complex, as the dynamics and radiation field influence the dust formation process and the amount of dust affects the dynamics and the radiation field. At the temperatures at which dust grains form, most elements are locked in molecules and at the densities of the inner wind a rich chemistry develops. The study of dust formation is the study of chemical pathways that take molecules from the gas to the solid-phase under the conditions of the extended atmospheres of AGB stars. However, theoretical predictions are not easily achieved, as many processes important in the dust formation, growth and processing are still poorly understood even under laboratory conditions. Furthermore, the formation of dust happens in a chaotic environment where pulsation-induced shocks, a varying stellar radiation field, and a large number of different chemical reactions play important roles. The fact that the timescales on which these processes modify the medium are comparable to those for grain growth makes the modelling of dust formation difficult. It is obviously necessary that models treat all the components simultaneously with time-dependent radiative transfer and dynamics. Because of this, no complete description of dust nucleation and growth has been possible yet.

Although most of the relevant processes possibly happen under non-equilibrium conditions, studying the chemical equilibrium between mixtures of gas and solids is an important tool to understand the dust species that likely form from ejected gas in the AGB circumstellar environment. This is a common problem of thermodynamics and consists of finding the minimum of the Gibbs energy with respect to all solid and
1 Introduction

Figure 1.5: Stability limits given in the pressure-temperature plane of minerals formed by the most refractory elements, Mg, Fe, Si, Al, Ca and of Ti and Zr. The chemical formulae of the minerals represented are: Al$_2$O$_3$ (corundum), CaTiO$_3$ (perovskite), Ca$_2$Al$_2$Si$_7$O$_{20}$ (gehlenite), MgAl$_2$O$_4$ (spinel), MgCaSi$_2$O$_6$ (diopside), Mg$_2$SiO$_4$ (forsterite), MgSiO$_3$ (enstatite), Fe (iron), and FeS (troilite). The dashed lines are $P-T$ trajectories that correspond to a $10^{-5}$ $M_\odot$ year$^{-1}$ AGB outflow (stellar wind) and the photosphere $\tau = 2/3$ (disc:photosphere) and the midplane (disc:midplane) of a stationary protoplanetary disc of a solar-like protostar with a $10^{-7}$ $M_\odot$ year$^{-1}$ accretion rate (from Gail 2010).

A more complex problem than finding stable solutions for gas-solid mixtures is to calculate which materials condense from a pure gaseous mixture of a given composition. The formation of solid particles in this condition is often regarded as a different process given its complexity. It is referred to as nucleation. Once the (tiny) seed nuclei are formed, the growth of dust species is enormously facilitated. The composition of the seeds and the grain that grows around it can (and likely do) differ. Dust nucleation in the outflows of carbon-rich stars is much better understood than in oxygen-rich environments because of important contributions of data from industry on modelling of terrestrial flames. In oxygen-rich environments, nucleation is still an
open problem but some progress has recently been made from quantum mechanical calculations, especially on cluster structures (e.g. Jeong et al. 2000; Chang et al. 2000).

Another complicating factor for the study of oxygen-rich environments arises from the fact that dust mixtures consisting of oxides might suffer from solid diffusion or solid-state chemical reactions, which alter their composition. Also, the lattice structure of oxygen-rich dust has a very strong effect on the optical properties of the dust. The structure of newly formed dust in astrophysical conditions is expected to be amorphous (with a disordered structure) in most cases but if exposed to high enough temperatures, the building blocks rearrange themselves in more energetically favourable (regular) crystalline structures. The process of changing a solid from an amorphous to crystalline structure is called annealing and an example of the time scales involved are given in Fig. 1.6. All these processes are time-dependent, not completely understood, and occur in the chaotic environments of the outer atmospheres of AGB stars. For carbon-rich stars, the observed data obtained so far can be explained with simpler models that do not require dust processing but dust processing is likely also important for these sources.

Another important distinction in dust formation in the circumstellar envelopes of AGB stars is with respect to whether the opacity provided by the formation or growth of dust grains is added before or after the wind has been launched. If we ignore the momentum input due to radiation pressure on molecules, shocks and magnetic fields, a simplified condition for a dust driven wind is that radiation acceleration on dust grains exceeds gravity. The ratio between these two forces, Γ, is

\[ \Gamma = \frac{\kappa L_\ast}{4\pi cGM_\ast} \]

where \( \kappa \) is the “fluxed averaged mean opacity”, \( L_\ast \) and \( M_\ast \) the luminosity and mass of the star, and \( c \) and \( G \) the speed of light and the gravitational constant. The “flux averaged mean opacity” is the opacity of the given dust species averaged over the incident flux and integrated over the grain size distribution function. It can be very difficult to calculate as direction dependent scattering can account for an important fraction of the total opacity and is strongly size dependent.

Calculations of isothermal winds, for which an analytical solution exists, lead to important qualitative conclusions that are still valid when dealing with more complex winds. These calculations show that winds will develop if the condition \( \Gamma > 1 \) is fulfilled at some point of the atmosphere. For a spherically symmetric wind, the radius at which the radiation pressure on the dust grain surpasses gravity is referred to as the critical point, \( r_c \). The mass-loss rate, \( \dot{M} \), is defined by the density, \( \rho_c \), and expansion velocity, \( u_c \), at \( r_c \) from the equation of conservation of mass, \( \dot{M} = 4\pi\rho_c u_c r_c^2 \). For a given stellar atmosphere, increasing the dust opacity below \( r_c \) forces
Figure 1.6: Timescales for annealing of a $0.1 \, \mu$m particle and for nucleation of enstatite (full lines). The timescales for vertical and radial transport in protoplanetary discs and the hydrodynamic timescale, $r/\nu$, of a stationary outflow are shown for comparison. Figure taken from Gail (2010).

the critical point inwards, to higher density regions, and leads to higher mass-loss rates. Increasing the dust opacity for $r > r_c$ does not affect the mass-loss rate but only the maximum expansion rate or terminal velocity of the outflow.

The molecular wind

The gaseous component in the outflows of AGB stars is mostly molecular and many molecules already form in the extended atmospheres. Even though the gas accounts for most of the mass (at least $\sim 99\%$), it is mainly only dragged by the dust grains. As they stream away, the molecules are exposed to different temperatures, densities, and radiation fields. A multitude of reactions takes place in the outflow, making the molecular composition of the wind a strong function of radius. Some of the reactions are important for further grain growth while others require a solid surface to take place. Models which take as input the atmospheric chemical composition and the coefficients of reaction rates are able to predict the radial abundance of molecules for different stellar and wind parameters (e.g. Willacy & Millar 1997; Cherchneff 2006).
To illustrate the complexity, we show a small set of the chemical reactions involving sulfur in Fig. 1.7. These depict the processes involving sulfur, oxygen, and hydrogen that are relevant in the inner wind of an oxygen-rich source (Willacy & Millar 1997). The inner wind abundances of these sulfur-bearing molecules are also affected by reactions with other elements not shown in the figure and many other reactions also have an effect on these abundances in an indirect way.

As the wind expands, the densities and temperatures decrease and the rates of the different reactions change, leading to the destruction or production of the different molecules. When the densities reached are too low, at large distances from the star, the reaction rates drop strongly and expansion continues without significant chemistry taking place. The fate of these molecules is to be dissociated in the outer parts of the molecular envelope by the interstellar radiation field. The abundances as a function of radius of the molecules involved in the reactions in Fig. 1.7 are shown in Fig. 1.8 (Willacy & Millar 1997). These chemical models depend on data on reaction rates that might be poorly known, or not at all, for the conditions encountered in the outflows of AGB stars. Observations of molecular abundances as a function of radius are extremely important to corroborate or constrain the results obtained. In Chapters 2 and 3, we calculate such models for CO, SiO, and H$_2$O for W Hya and in Chapter 5 for CO and SiO for R Dor and R Cas.
1 Introduction

Figure 1.8: Abundances of sulfur-bearing molecules involved in the reactions given in Fig. 1.7 as a function of radius (Willacy & Millar 1997).

1.6 Observations of circumstellar envelopes

Observations of AGB stars give important information to support theoretical efforts to understand the processes happening in these objects. Observations of the inner wind and atmospheres can reveal the conditions in the regions from where the wind is launched, and give insights into the mass-loss mechanism, while data on molecular and dust emission from the intermediate region of the wind constrain their chemistry and physical structure. Furthermore, a given circumstellar envelope encloses the mass-loss history of its parent AGB star, as the material that slowly merges into the interstellar medium carries information about the time at which it was ejected. This ‘memory’ can be lost due to interactions with the interstellar medium or with previously ejected matter. Nonetheless, studies of the circumstellar envelopes have shown strong mass-loss variations on scales of thousands and even hundreds of years (e.g. Decin et al. 2007; Schöier et al. 2011b; Justtanont et al. 2013; de Vries et al. 2014, Chapter 4) that are not always understood on the basis of present-day theoreti-
1.6 Observations of circumstellar envelopes

1.6.1 The dust

The dusty component of the circumstellar environment of AGB stars is studied in the vast majority of cases by analyzing its interaction with radiation. Important findings also come from research of the properties of pre-solar grains which are retrieved from meteorites and that are thought to be produced in AGB stars (from their isotopic signature) and to have survived the formation of the solar system (e.g. Nguyen et al. 2010; Takigawa et al. 2014). However, these grains are very few in number.

The grains in the circumstellar environments of AGB stars interact with the available photons either by scattering or absorption. The absorbed photons are converted into thermal energy of the grain. The grains emit radiation in the infrared and the balance between energy absorbed and irradiated sets the temperature of the particles. The radiation is more easily emitted or absorbed by grains in frequencies in which their constituent molecules are allowed to resonate, causing characteristic bands in the spectrum. One important point to note is that amorphous and crystalline dust have very distinct spectral characteristics, because of their different lattice structures. On the one hand, crystalline dust species show sharp, well-defined dust features that reflect the ordered structure of the lattice. On the other hand, the structure of amorphous dust is chaotic and when the many slightly different resonance frequencies are combined they result in broad spectral features.

The scattering, absorption and emission of light by dust grains are studied by different techniques and at different wavelengths both from the ground and from space. For scattering, images of visible light can reveal large dust shells produced by continuous mass loss over thousands of years (e.g. Mauron & Huggins 2000, 2006), or by intense mass-loss periods (e.g. González Delgado et al. 2003b; Maercker et al. 2010) which are often associated with thermal pulses (e.g. Olofsson et al. 1996; Mattsson et al. 2007). Polarimetric interferometry in the near-infrared can probe the innermost regions of the outflows. This technique was used to show the presence of large grains associated with the wind driving in oxygen-rich AGB stars Norris et al. (2012). In Chapters 4 and 5 we use these observations to constrain the masses of the halos of scattering grains around WHya, R Dor, and R Cas.

For the chemical and physical structure of dust species to be identified, infrared spectra are needed as most of the radiation emitted by solid particles is produced in this wavelength range. Because of the earths atmosphere, these spectra must be obtained mostly from space with instruments onboard satellites like IRAS, ISO, Spitzer, AKARI and Herschel. Observations from the ground are also possible in the atmospheric windows but do not provide nearly as much wavelength coverage and quality as those secured from space. Thermal dust spectra reveal characteristic features that
are compared to laboratory measurements of optical properties of solid materials. The variety of obtained spectra is vast with well-characterized differences between oxygen-rich and the carbon-rich sources and even hybrid objects (see Fig. 1.9). As shown in Fig. 1.10, a great diversity is also seen in optical depth with optically thin and optically thick dust emission arising from sources with low ($\sim 10^{-7} \text{M}_\odot \text{year}^{-1}$) and high ($\sim 10^{-5} \text{M}_\odot \text{year}^{-1}$) mass-loss rates. The higher mass-loss rate objects possess winds so optically thick that the central star becomes completely obscured. For these sources a direct study of the stellar spectrum is not possible and properties of the star have to be inferred.

In order to successfully determine the properties of the circumstellar dust, a library of optical constants of astrophysically relevant species is required. As the amount of pre-solar grains available is not enough to extract optical information, data must come from the dust species found on Earth or those synthesized in laboratories. Measuring the optical properties of these solids is difficult and the number of possible compositions vast. Hence, despite large efforts (e.g. Begemann et al. 1997; Jäger
1.6 Observations of circumstellar envelopes

Figure 1.10: ISO short-wavelength spectrometer spectra of oxygen-rich AGB stars with envelopes that have different optical depths (from Sylvester et al. (1999)).

et al. 2003; Hofmeister et al. 2009; Speck et al. 2013), optical properties of materials of many different chemical compositions and structures are still unknown.

The study and identification of dust features in astrophysical objects consists of comparing calculated models to the observed spectra. Such models can be simple, e.g. they may consist of only the opacity of the sample dust, or complex, involving full radiative transfer models that calculate the spectra for a given spatial distribution and opacity. The code used to model the dust emission of WHya, R Dor, and RCas, MCMMax (Min et al. 2009), is an example of the second approach. It solves the continuum-opacity radiative transfer problem using a Monte Carlo approximation (see Chapters 2, 3, 4, and 5). In order to calculate dust opacities, however, a dust particle model has to be adopted. The dust grain models most commonly used assume spherical particles (Mie theory, Mie 1908) or a distribution of shapes, such as
ellipsoids or hollow spheres (Bohren & Huffman 1998; Min et al. 2003). The latter approximations are thought to better reproduce the opacity of cosmic dust.

1.6.2 The gas

Molecular emission and absorption are by far the main sources of information on circumstellar gas. The emission is mostly produced from allowed transitions between quantized rotational, vibrational, or electronic energy levels. The interpretation of observed data becomes increasingly difficult for more complex molecules (with many atoms or a non-linear structure) with a large number of allowed transitions. The observations can be roughly divided in absorption lines against the bright stellar-continuum in the near-infrared and emission lines at mid-infrared and longer wavelengths. They come from molecules present close to the star, in the high-density medium of the extended atmosphere (Tsuji et al. 1997), up to the farther regions of the molecular envelope. The molecule most widely used for the study of the circumstellar environments is CO (e.g. De Beck et al. 2010; Justtanont et al. 2013; Ramstedt & Olofsson 2014), as it is ubiquitously present in high abundances in the entire molecular envelope and has a simple structure of its energy levels. Other studied molecules include SiO, H$_2$O, OH (e.g. González Delgado et al. 2003a; Maercker et al. 2009), found in large abundances around oxygen-rich sources, CN, CS, and HCN for carbon stars (e.g. Cernicharo et al. 2011; Schöier et al. 2013), and a combination of both in S-type stars (e.g. Danilovich et al. 2014). An example of a far-infrared spectrum full of molecular lines is given in Fig. 1.11. The spectrum of the oxygen-rich star W Hya was obtained with PACS onboard Herschel. Most of the transitions seen are associated with water, a smaller fraction is due to CO emission.

Despite the well-established dichotomy between carbon- and oxygen-rich stars, molecules that contain oxygen (such as H$_2$O and SiO) are observed with lower abundances around carbon-rich sources. The same happens for carbon-bearing molecules (such as HCN) around oxygen-rich sources. The reasons for this are thought to be traced back to the dissociation of CO molecules at the base of the envelope due to shocks (Cherchneff 2011), a deep penetration of UV photons because of a clumpy medium (Decin et al. 2010a), or both.

The absorption or emission signature of a population of a given molecule can be calculated from radiative transfer models based solely on its excitation structure and spatial distribution. However, obtaining the excitation structure for a molecular species in the outflow of an AGB star is not a simple task, not even when spherical symmetry is assumed. The levels are populated by collisions (mainly with H$_2$ molecules), direct stellar radiation, and radiation from dust, the considered molecular species, and possibly other molecules. Radiation produced in different parts of the envelope might affect excitation in distant regions, given the relative velocities (and
1.6 Observations of circumstellar envelopes

Figure 1.11: The PACS spectrum of W Hya with a large number of water and CO transitions that give important information on the properties of the envelope (see Chapters 2 and 3).

consequent Doppler shifts) and the highly direction dependent optical depths. To solve the complex problem of determining the level populations, numerical codes are necessary. GASTROoNoM (Decin et al. 2006, 2010b), used to model the molecular emission of W Hya in Chapters 2 and 3 and of R Dor and R Cas in Chapter 5, is one of such codes. The exercise might still be impossible, presently, for specific molecular species if data on collisional and radiative coefficients are not well constrained or unknown.

Studying different transitions and/or several molecular species may give complementary information on the derived envelope parameters. Typically, the higher the excitation energy of the upper level of a given transition, the closer to the star it will be excited. However, this is not a strict rule as, for example, the excitation of transitions can be strongly influenced by the non-local radiation field. On the one hand, for a given molecule whose excitation is coupled to the local gas conditions (as is usually the case for $^{12}$C$^{16}$O), transitions with progressively lower excitation energy will probe material at increasingly larger distances from the central star. On the other hand, different molecules can be sensitive to different parameters either due to stronger intrinsic transition coefficients, different abundances, or distinct spatial distributions. Therefore, including many transitions of different molecules in the study of the molecular envelope of AGB stars sets stronger constraints on the derived
properties.

Observations that spectrally or spatially resolve the emission in a given transition provide further, unique constraints on the envelope properties (e.g. Lucas et al. 1992; Schöier et al. 2004, 2011b; Maercker et al. 2012). Spectrally resolved observations give information on the velocity structure of the envelope as they reveal the Doppler broadening caused by the expansion of the envelope (of typically \( \sim 10 \text{ km s}^{-1} \)). If such observations are performed for transitions excited both close and far from the star, the acceleration of the envelope can be probed. Observations of this kind help unveil the wind acceleration mechanism (e.g. Cernicharo et al. 2010; Decin et al. 2010c; Schöier et al. 2011a; Justtanont et al. 2012; Danilovich et al. 2014). Spatially resolved observations are capable of constraining the regions in the envelope from where emission of a given transition originates. Hence, they probe the density and temperature structure of the envelope and help to break degeneracies between these two properties. With the advent of ALMA, observations have revealed structures and asymmetries that are far too detailed to be reproduced by the spherical-symmetrical molecular-radiative-transfer codes mostly used at present (e.g. Vlemmings et al. 2013).

1.6.3 Variations in the mass-loss rate

The total mass lost during the AGB phase clearly depends on initial stellar mass, since all AGB stars are reduced to white-dwarves of similar masses (of \( \lesssim 1 M_\odot \)) but have very different masses at the beginning of the AGB (ranging from 0.8 to \( 8 M_\odot \)). However, the evolution of the mass loss for a stars of a given initial mass is not yet known. When measuring mass-loss rates from molecular line emission or dust infrared excess, only the mass loss from up to tens of thousands of years ago is probed. Because of this only mass-loss variations on timescales \( \lesssim 10^5 \) years can be measured for an individual star. Changes in the mass-loss rate over larger periods of time have to be inferred from studies of a large number of sources. In these samples, variations of the mass-loss rate due to other parameters and due to the evolution time on the AGB are difficult to disentangle. Besides variations on the mass-loss rate caused by the evolution on the AGB of a single star, differences in the mass-loss rate are also expected to be seen for different stellar luminosity, mass, and temperature (Olofsson 2003).

Due to the large uncertainties usually associated with distance estimates for AGB stars in our galaxy, the dependence of mass-loss rate with luminosity is better studied by using sources in the Magellanic clouds, for which the distance is well-known (Lattanzio & Wood 2003). A study by (Srinivasan et al. 2009) shows that the luminosities and infrared excess of the oxygen- and carbon-rich AGB stars observed correlate. The correlation is particularly good for the objects with strong dust emission. It shows a
lot of scatter, however, for sources with low luminosities, below $\sim 3 \times 10^4 \, L_\odot$. This suggests that the mass-loss rate of AGB stars in the lower luminosity range depends strongly on other parameters.

As shown in Fig. 1.12, it is well-establish that the mass-loss rate also correlates with pulsation period. The main cause of this is thought to be the dependence of pulsation period with envelope mass. The complete explanation is undoubtedly more complex, as stars with similar periods but different pulsation properties are sometimes observed to have different mass-loss rates (Olofsson 2003).

Shells produced by mass-loss rate peaks associated with thermal pulses are also seen around AGB stars (e.g. González Delgado et al. 2003b; Maercker et al. 2010, 2012). The shells are seen in both CO emission and scattered light and only around carbon-rich sources. The mass-loss rates observed during the thermal pulses are of up to two orders of magnitude higher than the inter-pulse mass loss. Although the high-mass-loss-rate phase is short ($\sim 100$ years) it has an important contribution to the total mass lost. Mass-loss rate variations with timescales of hundreds or thousands of years are also measured but no definitive explanation has been given for this modulation.

**Figure 1.12:** Mass-loss rates and period for oxygen-rich stars (left panel) and carbon-rich stars (right panel). Semiregulars (diamonds), Miras (circles), and Galactic Center OH/IR-stars (squares) are shown (from Olofsson 2003).
For example, evidence suggests that the high mass-loss rate outflows from several OH/IR stars are only about a thousand years old (Justtanont et al. 2013; de Vries et al. 2014). For lower mass-loss rate sources, variability on short timescales also seems to be conspicuous as many sources show important changes on the mass-loss rates on timescales of $\sim 10^2$ to $10^3$ years (e.g. Marengo et al. 2001; Decin et al. 2007; Schöier et al. 2011b, Chapter 4).

1.6.4 The Herschel observatory

Recently, the launching of the Herschel Space Observatory (shown in an artistic impression in Fig. 1.13, Pilbratt et al. 2010) has revealed many new molecular transitions never detected before and shown details of the distribution of cold dust in many different astronomical sources. This new data has already significantly helped advance our understanding of the AGB envelopes but, due to the immense amount of information, much more is still to be learned from further analysis observations. The mirror of Herschel is 3.5-metres in diameter and is the largest ever sent to
space. Its instruments cover the far-infrared and sub-millimetre spectral range (55 to 672 µm), a large part of which was unexplored. Observations made from the ground cannot access a large fraction of this wavelength range due to restrictions inflicted by the Earth’s atmosphere. In particular, many transitions of the water molecule (ubiquitously present in the universe, including our atmosphere) were observed and studied for the first time with the satellite.

Due to the spectral region of interest, the detection system has to be cooled to temperature as low as 0.3 K. The over two thousand litres of liquid helium required for the effective cooling to these low temperatures is what set the mission lifetime of slightly more than three years. While the liquid helium supply lasted, the three instruments onboard Herschel, the Heterodyne Instrument for the Far Infrared (HIFI; de Graauw et al. 2010), the Photodetector Array Camera and Spectrometer (PACS; Poglitsch et al. 2010), and the Spectral and Photometric Imaging Receiver (SPIRE; Griffin et al. 2010), collected unprecedented data on a vast number of infrared sources in the sky. The instruments are complementary not only in wavelength coverage but also in capabilities. The very high spectral resolution (as high as $10^7$) of HIFI provides spectrally resolved lines in the range 157 - 625 µm, revealing details of velocity structure of the winds of AGB stars. PACS and SPIRE produced spectra with a large wavelength coverage and hundreds of transitions detected in a single pointing. Although the transitions from AGB stars are not spectrally resolved by these two instruments (spectral resolution is less than ~3000), the amount of information collected over a broad range of excitation energy reveals not only many transitions never measured before but also many lines that have yet to be identified (see Chapter 2). Another observing mode of PACS and SPIRE is the imaging photometry mode, which provided simultaneous images in bands centered at 70 µm or 110 µm together with 160 µm for PACS and 250, 350, and 500 µm for SPIRE.

Most of the data used in the studies included in this thesis were obtained in the context of the guaranteed-time key programmes: HIFISTARS (for HIFI, PI Bujarrabal, V.) and MESS (Groenewegen et al. 2011, for PACS and SPIRE).

1.7 This thesis

The gaseous and dusty parts of the circumstellar medium of AGB stars are frequently studied separately. Because of this, very few models exist that provide a comprehensive picture of the outflow of individual targets. Nevertheless, these two components affect each other and models that take both the gas and the solid phases into account are able to set more stringent constraints on the derived parameters.

The studies included in this thesis concern the investigation of the circumstellar envelope of AGB stars in a comprehensive way (gas and dust modelled simultane-
Introduction

ously). For that, we use a large number of observed molecules and transitions to trace the gas, and several different data of distinct character to unveil the dust. By properly understanding individual objects in-depth, and in their complexity, we aim to uncover processes and features that are important in the lives and evolution of AGB stars in general. Our goal is to study both components of the circumstellar envelope to obtain a consistent picture. We are specially interested in tracing dust forming elements in the gas and solid phases. The objects of study belong to one specific sub-class of AGB stars, low-\( \dot{M} \) oxygen-rich objects, and we focus mainly on one source: \textit{W Hya} (Chapters 2, 3 and 4). The work presented here is primarily driven by one question: what drives the wind of low mass-loss rate oxygen-rich AGB stars? For this, we investigate the region where the wind is accelerated, the structure of the flow, and the past mass-loss rate and overall properties of \textit{W Hya}.

We characterize the outflow of \textit{W Hya}, deriving physical and chemical parameters for both the wind and the central star. The line shapes observed with HIFI allow for a detailed model of the velocity structure (Chapter 2 and 3), while the derived isotopic ratios constrain the initial mass of \textit{W Hya} when compared to evolutionary calculations (Chapter 3). In Chapter 4 we obtain a dust model in the light of the gas model obtained in Chapters 2 and 3. In order to achieve this, we advocate the need of a gravitationally bound dust shell from where most of amorphous \( \text{Al}_2\text{O}_3 \) emission originates. Our best model dust envelope is compared to observations of dust emission that probe the mass-loss rate thousands of years back and we obtain the recent mass-loss history of \textit{W Hya}. We also study the interface between the wind and the gravitationally bound dust shell using scattered light observations. In Chapter 5 we zoom out from \textit{W Hya} and look at the sample of low-\( \dot{M} \) oxygen-rich sources observed by HIFI. We successfully apply the model structure obtained for \textit{W Hya} to the other two sources that also present significant amorphous \( \text{Al}_2\text{O}_3 \) emission: \textit{R Dor} and \textit{R Cas}. We compare the three sources looking for similarities and differences that shed light on the wind driving-mechanism of low-\( \dot{M} \) oxygen-rich AGB stars.

There is still much to be learned about how the lives of low- and intermediate-mass stars end. The work presented here is based on unprecedented data acquired with Herschel, it touches many of the aspects of these winds and shows that there is still much to be revealed from the exquisite observations obtained with this satellite. The results obtained raise important questions about the connection between the observed infrared spectrum and the commonly assumed distribution of dust around AGB stars. Moreover, we find that important conclusions can be drawn based on the consistent study of the gaseous and solid components of the wind of individual sources.