Bow-shock chemistry in the interstellar medium
Ngoc Tram Le

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Chimie des chocs d’extrave dans le milieu interstellaire

Ecole doctorale 127
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Declaration of Authorship

I, LE NGOC TRAM, declare that this thesis titled, ’BOW-SHOCK CHEMISTRY IN THE INTERSTELLAR MEDIUM’ and the work presented in it are my own. I confirm that:

- This work was done wholly or mainly while in candidature for a doctoral degree at Observatoire de Paris.
- Where any part of this thesis has previously been submitted for a degree or any other qualification at Observatoire de Paris or any other institution, this has been clearly stated.
- Where I have consulted the published work of others, this is always clearly attributed.
- Where I have quoted from the work of others, the source is always given. With the exception of such quotations, this thesis is entirely my own work.
- I have acknowledged all main sources of help.
- Where the thesis is based on work done by myself jointly with others, I have made clear exactly what was done by others and what I have contributed myself.

Signed: 

Date: 

______________________________
For my mother MA Thi Kieu, my younger sister LE Thi Ngoc Tram and my family ...
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Stars are bad neighbors: they often disturb their surroundings. They sometimes travel very fast through the interstellar medium (ISM). They frequently undergo violent ejection events which leave an imprint on their neighborhood (jets, winds, supernovae). These supersonic flows generate shocks both in the ejected material and in the stellar environment. The study of these shocks constitute the subject of this thesis, and we model them with the Paris-Durham planar shock code, which incorporates a wealth of micro-physics and chemical processes relevant to the magnetized ISM.

First, we use this code to model 3D magnetized axisymmetric bow shocks with arbitrary shapes, thanks to a formalism which links mathematically the shape of shocks to an equivalent statistical distribution of 1D shocks. For the first time, we examine systematically the effect of the geometry, age, and various other parameters on the H$_2$ excitation diagram and emission line profiles. For example, we unveil a geometrical effect which shows that 1D planar shocks emission fits to 3D bow shocks are biased towards small velocities. We also apply our models to spatially integrated H$_2$ observations of bow-shocks in Orion BN-KL and BHR71 where a much better match is obtained with only a limited number of additional parameters compared to former planar models. We illustrate on the Herbig-Haro object HH54 how spectrally resolved H$_2$ line emission profiles can be used to extract a wealth of dynamical information.

Second, we include in the Paris-Durham shock code a minimum set of processes necessary to describe asymptotic giant branch (AGB) wind models: geometrical dilution, external interstellar radiation, radiative pressure on grains, gravity, heating from stellar radiation pumping, three-body reactions, and sonic-point crossing. With this tool, we started to examine the time-dependent chemistry of hydrogen in winds of hot and cool AGB stars. We suggest that the low abundance of HI inferred from observations is due to hydrogen locked in its molecular form, and we use our model to try and reproduce HI line observations lines in a hot AGB (Y CVn) and a cold AGB (CW Leo).

Although we have mainly focused on atomic or molecular hydrogen in this study it would be straightforward to extend it to other molecules with optically thin transitions. These simplified tools to model chemistry for complex geometries and dynamics are proving
very useful at a time when new instruments such as ALMA discover a wealth of spectral and spatial information for a multitude of chemical tracers, and also when the JWST will soon provide complementary data in the infrared H$_2$ and ionic lines with unprecedented resolution and sensitivity.
École Doctorale d’Astronomie et d’Astrophysique d’Île de France

Résumé français

CHIMIE DES CHOCS D’ÉTRAVES DANS LE MILIEU INTERSTELLAIRE

Les étoiles sont de très mauvaises voisines: elles perturbent souvent leur environnement. Parfois, elles se déplacent à grande vitesse dans le milieu interstellaire (MIS). Souvent, elles subissent des soubresauts violents qui laissent une empreinte dans leur voisinage (jets, vents, supernovae). Ces flots supersoniques génèrent des chocs à la fois dans le matériau éjecté par l’étoile et dans l’environnement stellaire. L’étude de ces chocs constituent le sujet de cette thèse, et nous les modélisons avec le code de chocs stationnaires plan parallèle Paris-Durham, qui incorpore une riche panoplie de processus microphysiques et chimiques adaptés au MIS magnétisé.

Tout d’abord, nous utilisons ce code pour modéliser des chocs magnétisés 3D pour des formes arbitraires à symétrie axiale, grâce à un formalisme qui lie mathématiquement la forme des chocs à une fonction de distribution de chocs 1D équivalente. Pour la première fois, nous examinons systématiquement l’effet de la géométrie, de l’âge, et de quelques autres paramètres sur le diagramme d’excitation de H$_2$ résultant et la forme des profils raies d’émission de H$_2$. Par exemple, nous dévoilons un effet géométrique qui montre que l’ajustement par des modèles 1D de l’émission de H$_2$ observée sur un choc 3D est sujette à un biais vers les basses vitesses. Nous appliquons aussi nos modèles à l’observation de H$_2$ spatialement intégrée de chocs d’étrave dans Orion BN-KL et BHR71 où nous obtenons un bien meilleur ajustement des observations avec un nombre à peine plus grand de paramètres comparé aux modèles précédents. Nous illustrons sur l’objet de Herbig-Haro HH54 la grande richesse d’information dynamique que renferme le profil des raies d’émission résolues de H$_2$.

Ensuite, nous incluons dans le code de Paris-Durham un ensemble minimal de processus nécessaires pour décrire les modèles de vents d’étoiles de la branche asymptotique des géantes (AGB): la dilution géométrique, l’irradiation externe, la pression de radiation sur les grains, la gravité, le chauffage dû au pompage radiatif par l’étoile, les réactions à trois corps et le passage du point sonique. Avec cet outil, nous commençons à examiner la cinétique chimique de l’hydrogène dans les vents d’étoiles AGB chaudes et froides. Nous suggérons que la faible abondance de HI déduite des observations s’explique par la forme principalement moléculaire que prend l’hydrogène. Nous générions le choc terminal dans le vent et nous essayons avec nos modèles de reproduire les observations de la raie HI dans une AGB chaude (Y CVn) et une froide (CW Leo).
Bien que nous ayons principalement concentré notre attention sur l’hydrogène (atomique ou bien moléculaire) dans cette étude, l’extension de ce travail à des transitions optiquement minces d’autres molécules est assez directe. Ces modèles simplifiés pour modéliser la chimie dans des géométries et dynamiques néanmoins complexes se révèlent très utiles au moment où de nouveaux instruments comme ALMA dévoilent une grande richesse spectrale et spatiale pour une multitude de traceurs chimiques. Ceci alors que le JWST est sur le point d’apporter dans l’infra-rouge de l’information complémentaire sur les raies de H₂ et les raies ioniques avec une résolution et une sensibilité inégalées.
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Part I

INTRODUCTION
Chapter 1

INTERSTELLAR SHOCKS

1.1 Introduction

The gas in between stars is usually much colder than them. As a result of the slow velocity of sound, flows can easily become supersonic. The relative motions of stars or gaseous clouds can be sufficient to trigger shocks. On top of that, stars are subject to violent events during their life. Immediately after their birth, the gas which does not make it onto the surface can be ejected and impact the surrounding interstellar medium (ISM) through outflow cavities and protostellar jets. Later in their evolution, stars launch winds which can become supersonic very quickly with respect to their cold environment. At the end of their lives, some stars end up in a burst of supernovae ejecta which generate shocks at extremely large velocities. Finally, large scale galaxy collisions can also shake the gas supersonically and generate shocks. The interstellar gas inside galaxies is thus continuously permeated by traveling shock waves, which heat up and illuminate the gas. The emission of light, which can be observed by astronomers, gives us as many opportunities to access informations on the galactic dynamics.

1.2 Shock waves

A wave is a perturbation propagating in a fluid without changing. A shock wave is a pressure wave that moves faster than the speed of sound in that fluid. In nature, shock waves or simply shocks are common phenomena. In principle, an object will deflect the gas molecules when it penetrates through it. If the speed of the object is much smaller than the speed of sound, the density of gas remains approximately constant (Figure 1.1, top). If it is comparable (but lower) to the speed of sound, its motion is always behind
the sound wave launched from the previous position (Figure 1.1, bottom left), and the gas is swept away and its density is compressed by the object. This compressive gas flow is then nearly reversible and its properties are well described by the isentropic condition, with entropy remaining constant. When the object moves faster than the speed of sound, all the compressive waves sent ahead to sweep the gas are caught up by the object, and gathered in an abrupt structure: a shock wave is formed (Figure 1.1, bottom right) with an opening angle of the cone $\mu$. This angle allows us to estimate the speed of the supersonic motion through the Mach number ($M$), defined as $M = v/c_s$ with $v$ and $c_s$ the speed of the object and the speed of sound. The opening angle of the cone satisfies
\begin{equation}
\sin(\mu) = \frac{c_s}{v} = \frac{1}{M}.
\end{equation}
Unlike sound waves, shock waves are non linear waves and they largely change the gas properties. Across the shock wave, the pressure, the density, the temperature and the entropy of the gas abruptly jump. Downstream, the kinetic and thermal energy of the gas in the shock wave dissipate rapidly with respect to the distance: a shock wave is an irreversible (or non-isentropic) process which dissipates kinetic energy into heat and radiation. If not sustained, a shock wave loses its energy over some distance as it heats gas and it degenerates into a conventional sound wave.

Typically, there are three types of shock waves around a moving solid object (Figure 1.2). A shock wave is called normal if its front is perpendicular to the direction of the entrance velocity. In this case, the flow direction does not change. However, during the motion of
Figure 1.4: Geometric condition of the supersonic object in order to form a bow shock. The bow shock is formed when the size-angle of the infinite-wedge object $\delta$ exceeds its maximum value at a given Mach number. $\theta$ is the angle of the oblique shock (Figure 1.2, middle panel).

the object, it may not remain perpendicular to the flow direction. When the shock wave front is inclined with respect to the flow direction, it is called an oblique shock. Oblique shocks are more easily generated by pointy parts of an object such as the nose, the edge of the wing, and the trailing edges of the supersonic plane shown in Figure 1.3. Oblique shocks are not always the preferred form around supersonic objects. If we consider a supersonic infinite-wedge object with size-angle $\delta$, the possible oblique shock is defined by the angle $\theta$ (Figure 1.2, middle), which differs from the supersonic angle $\mu$ above. At Mach number $M > 1$, the existence of the oblique shock around this infinite-wedge object can be determined via Figure 1.4 (more details can be found in the lecture of Daniel Guggenheim School of Aerospace Engineering¹). For example, if the object is moving with $M = 3$, and its size-angle is larger than $34^\circ$, there is no oblique shock around it. In this case, the solution is a bow shock (or detached shock), which sits ahead and does not attach to the object (Figure 1.2, right). Bow shocks cover all ranges of oblique shocks from the strongest normal shock at the centerline and to weaker shocks in the curving wings of the bow. In practice, bow shocks need to be considered in the design for return.

¹http://seitzman.gatech.edu/classes/ae3450/outline.html
capsules from space missions (Figure 1.5) for two reasons: (1) the drag of the capsule in supersonic motion is significantly increased by the surrounding bow shock; and (2) the capsule is not directly in contact with the bow shock, so that its temperature is kept below the melting point.

1.3 Astrophysical shocks probe stellar evolution

In astrophysics, shocks are ubiquitous. They form at three stages in stellar evolution: at early stages, when stars are born, shocks are formed by the interaction of young stellar objects outflows with the ISM; at near the end of the lives of low- and intermediate-mass stars, stellar winds produce shocks; and at the end of the life of high mass stars, the supernova phase generates extremely high velocity shocks.

This mass loss behavior leads to chemical enrichment of galaxies, reprocessing of matter, and generation of turbulence; it also influences star-formation processes, and thus impacts the further evolution of stellar systems and galaxies.
**Figure 1.6:** Stellar evolution diagram. *Left* Evolution of a low-mass star. *Middle* Evolution of an intermediate-mass star. *Right* Evolution of a high-mass star.

### 1.3.1 Early stellar evolution and outflow shocks

In general, stars form in dense molecular regions such as the cores inside the interstellar clouds, which contain gas and dust. At some point, these regions cannot resist their own gravity and they collapse. While collapsing, the density of the core increases, the inner region becomes optically thick, and the core is heated by the released gravitational energy. Once more material concentrates on the center, the increasing pressure stops the free fall to the central point and the core reaches a quasi-hydrostatic equilibrium, thus forming a protostar. Gradually, the envelope matter is depleted by accretion processes onto the new stellar surface. The protostar is further heated by the released gravitational energy. There, the thermal energy is converted into radiant energy that contributes to the luminosity of these objects. The angular momentum of the collapsing envelope is reduced by magnetic breaking the ejected outflow along the polar direction of the protostar, as confirmed by observation (e.g., Konigl and Pudritz 2000). The first model of outflow was derived by Snell et al. (1980) who discovered 2 lines of CO from a large molecular outflow in the L1551. Figure 1.7 shows two outflows in opposite directions, the outflow sweeps out most of the ambient gas into a dense shell supported by the strong stellar wind and the shell itself also moves through the molecular cloud.

Since then, many observational evidences of outflows have been observed in young stellar objects with higher resolution (http://casa.colorado.edu/hhcat/). These outflows have supersonic motion and are driven by jets, which are narrow and difficult to detect. However, supersonic jets interact with the surrounding ambient medium and create one of the most beautiful astrophysical phenomenon: a shock (see section 1.2). These shocks are easier to detect and to observe, and their properties allow us to deduce the properties of jets or
even further of the protostar. Figure 1.8 displays the bipolar jet from the Herbig-Haro object HH212 in the Orion cloud. The left side panel shows an infrared image observed by the ground telescope of the European Southern Observatory (ESO). The right side panel shows the map of 2.12 μm H₂ emission, captured by the Infrared Astronomical Satellite (IRAS) (Zinnecker et al. 1996). One can see the bipolar structure of the jet traced by the shock-excited rovibrational v=1-0, J=3-2 line of molecular hydrogen. This delineated bipolar structure is an important tool for revealing protostars. First, it allows us to determine their locations, where they are obscured, due to the drop of gas and dust density away from the source (McCaughrean et al. 1994). Second, it allows us to determine the proper motion of the jet without using another reference star (e.g., McCaughrean et al. 2002, Correia et al. 2009).
1.3.2 Low and intermediate mass late stellar evolution and shocked wind

When the temperature of a protostar exceeds $8 \times 10^6$ K, hydrogen fusion reactions start. Hydrogen is burnt into helium and energy is released out. Then stars begin their life on the main-sequence. After central hydrogen is exhausted, the helium core shrinks, and is heated again by the released gravitationally energy. The hydrogen is then continuously burnt, surrounding an inactive helium core. During this stage, the star approaches the red giant branch (RGB). From this point on, the lifetime and shock strength depend on its initial mass.

Low-mass stars ($M_i \leq 2M_\odot$): fusion gradually exhausts hydrogen during stellar evolution in the main-sequence, but hydrogen burning still continues in a thick shell, moving outwards through the envelope. The still dormant helium core becomes electron degenerate and remains continuously fed by additional helium from that hydrogen burning shell. As the degeneracy sets in during the main-sequence phase, the temperature of the helium core is minimum, close to the surrounding H burning shell. Then the temperature
decreases due to the degenerate electrons. The star globally starts to expand its own envelope. The He-core becomes denser, but the temperature did not reach yet the critical value required for helium fusion. During this phase, the luminosity increases drastically and the outer layers become convective. The convective region can reach down to the hydrogen burning shell, converted to helium and nitrogen via a CNO cycle. The newly formed elements are then mixed upwards to the upper layers through convection. This convection process mixing nuclear processed materials into the outer layer is called first dredge-up. It leads to the enrichment of the surface layers. Finally, the thermal pressure from fusion is no longer sufficient to counter the gravity. The stars start to contract and to increase in temperature until the stars eventually becomes compressed enough so that the helium core becomes highly electron degenerate. This degeneracy pressure is finally sufficient to stop further collapse of the most central material. When the temperature reaches around $10^8$ K, the helium ignites and starts to fuse at the center through the triple-alpha process, by which three $^4\text{He}$ nuclei transform into $^{12}\text{C}$ and other heavier elements, $^{16}\text{O}$, $^{20}\text{Ne}$, $^{24}\text{Mg}$. When the helium fusion begins with the triple-alpha process, the fusion rate raises rapidly, which again increases the temperature. This thermal run-away process is called He-core flash. However, the total pressure only weakly depends on the temperature, since the degeneracy pressure (which is only a function of density) dominates thermal pressure that is proportional to the product of density and temperature. Therefore, the steep increase in temperature only causes a slight increase in pressure, so that the core cannot cool by expansion. However, the run-away process can make the temperature quickly rises to the point that thermal pressure is again dominant, eliminating the degeneracy. From then on, the core can expand and cool down, maintaining temperature to the critical value of $10^8$ K, where stable He-burning starts. During the phase of core He burning, the central He supply gradually exhausts and an oxygen-carbon core develops. After the exhaustion of the central helium, the star evolves to the early asymptotic giant branch (AGB) phase. In this phase, the stellar luminosity of the star increases at almost constant temperature, and the stellar radius strongly increases. Surrounding the carbon-oxygen core is a helium-burning shell and a hydrogen-burning shell. These provide the energy output of the star. Above the He- and H-burning shells lies a deep convective stellar envelope (Figure 1.9). At this stage, most of the luminosity of the star is provided by the H-burning shell. From now, the evolution of the low-mass stars is similar to the intermediate-mass star. This entire process is displayed in Figure 1.6 (left).

Intermediate-mass stars ($2\ M_\odot < M < 8\ M_\odot$): due to higher mass, and hence higher temperature, a convective core has developed because the nuclear burning in the core is sensitive to the temperature. This convective core contracts as hydrogen converts to helium. After H-core exhaustion, the convective He core remains and the stellar envelope expands, but H-burning continues in a shell. In this phase, the first dredge-up also appears. From now, the star evolves upward on the red giant branch (RGB) at a nearly constant surface temperature, and its radius also increases. During this phase, the central He core
is contracting and heated by the gravitational energy. Again, when the central temperature exceeds $10^8 \ K$, the helium is ignited at the central region and forms carbon nuclei $^{12}\text{C}$ through the triple-alpha process and other heavier elements. Contrary to low-mass stars, the He-core has burnt under non-degenerate conditions, which avoids the He-core flash. After the ignition of helium, the star starts moving to the left on the Hertzsprung-Russel Diagram (HRD), to higher surface temperature and higher luminosity. When temperature at the center is lower than the critical value, the He core-burning stops but the He still continues to burn in the thick shell. The He-exhausted core again contracts and heats, while the hydrogen envelope expands and cools down. In the HRD, the star evolves again toward to the giant branch. The convective envelope penetrates the dormant hydrogen shell and mixes $^4\text{He}$ and $^{14}\text{N}$ upwards to the outer layers. This mechanism is called second dredge-up. The He shell burning heats up the base of the convective envelope and then makes the H burning to be reignited on top the He-shell. In the HRD, the star has reached the asymptotic giant branch (Figure 1.6, middle).

Since the He-shell is thin compared to the radius of the shell (Figure 1.9), its expansion...
**Figure 1.10:** Variation in surface luminosity (solid line), hydrogen-burning luminosity (dashed line) and helium-burning luminosity (dotted line) during a flash cycle for a $2M_\odot$ star (Wood and Zarro 1981).

**Figure 1.11:** Inner structure of an AGB and dredge-up process due to thermal pulse. There are two convective zones, which mix the nuclear products to the stellar surfaces during TP-AGB phase (Basso et al. 1999).
is essentially isobaric. The temperature of the shell, therefore, must increase. This makes the He-shell thermally unstable (Schwarzschild and Härm 1965). A slight increase in temperature leads to a steep increase in the release of the nuclear energy through triple-alpha process, which further increases the temperature since the shell is extending. This thermal run-away process is able to increase the luminosity of the He-shell upto $10^5 L_\odot$. Upon reaching the luminosity peak, the He-shell is widely extended and thermally stable. Then the whole region contracts again, the H-shell is reactivated, and the flash cycle is repeated. This increase in luminosity is referred to as He-shell flash or thermal pulse. The star, therefore, is now located on the thermally pulsing AGB phase (TP-AGB). The thermal pulse process is shown in Figure 1.10. During the TP-AGB phase, there are two convective zones: the inner convective zone is located in the intershell convection zone and mixes the processed matters from the He-shell (mainly $^{12}$C) upwards to the H-burning shell (Figure 1.11). After the He-shell flash and before the next shell flash, the outer convection zone reaches down to the intershell region and convects the material from this region upwards to the stellar surface. This mechanism enriches the newly processed matter from the inner region out to the outer envelope. This is called the third dredge-up. During this dredge-up process, $^{12}$C is enriched outward, and the C/O ratio increases from a value lower than 1 to a value higher than 1. Therefore, the third dredge-up is responsible for the formation of carbon-rich stars. The timescale of the star on AGB and TP-AGB phases depends on its initial mass and its metallicity. A star with $M_\ast = 1 M_\odot$ and $Z = 0.006$, for example, spends $\sim 10^7$ yr on the early AGB phase and $\sim 10^6$ yr on the TP-AGB phase (Rosenfield et al. 2014).
The star has lost most of its own mass during the AGB phase, mainly due to stellar winds that are supersonic, and therefore generate shocks when they interact with the ambient gas (Lamers and Cassinelli 1999). Figure 1.12 illustrates the shock created by the wind from an AGB star named IRC +10216 (Sahai and Chronopoulos 2010). The observation is performed by the Galaxy Evolution Explorer (GALEX) satellite in two wavelength ranges: 1344–1786 Å (near ultraviolet band - NUV) and 1771–2831 Å (far ultraviolet band - FUV). The asymmetry of the ring from east to west direction demonstrates that the IRC +10216 star moves eastward into the ISM. In fact, Figure 1.12 shows the emission of the extended ring in the FUV band that is not visible in the NUV band. The strong FUV emission ring delineates the shock caused by the interaction between the wind from IRC +10216 with the surrounding ISM rather than by the dust scattering. Three are two reasons: first, in the case of dust scattering, the FUV/NUV ratio is expected to be $\sim 2.4$ (Whittet 1992), where the observed value is $\sim 6$. Second, the collisional excitation of the molecular hydrogen with the electrons in the shocked gas is the mechanism that best produces detectable FUV radiation, but no detectable NUV radiation. The region between the ring and the star position is a freely expanding stellar wind (unshocked wind). In this region, the emission is seen in both the NUV and FUV bands due to the scattering of ambient galactic starlight on dust particle in the stellar wind.

After the thin nuclear active shell burning around the central core stops because the fuel supply runs out, the core of the star moves to the left on the HRD and can be observed as a planetary nebula. The star is then deceased. The remnant core becomes a white dwarf and cools down.

### 1.3.3 High mass late stellar evolution and supernovae shocks

**High-mass stars** ($M > 8 M_\odot$): the helium-core of such stars is ignited before they reach the RGB, which leads to the production of Fe, the strongest bound nucleus. Then, the stars no longer produce energy through fusion reactions and cannot hold up the gravitational forces any more. Eventually, electron captures on iron nuclei suppress the pressure support, with subsequent implosion and rebound leaving either a neutron star or a black hole, depending on the mass of the star (Figure 1.6, right).

The explosion of massive stars creates one of the brightest phenomenon in the Universe, known as supernovae. The huge energy ($\approx 10^{51}$ erg) produced by the explosion is able to create a tremendous shock in the surrounding medium (Nadyozhin 2008). 1987A is the brightest supernova blast observed from earth in more than 400 years (Figure 1.13). The shock velocity ranges from 300 to 1700 km s$^{-1}$ (Zhekov et al. 2006).
As we don’t have the tools to describe such powerful shocks, we will not hereafter study the shocks in supernovae remnants.

1.4 Jet-driven and stellar wind-driven bow shock models

1.4.1 Jet-driven bow shock configuration

The configuration of the jet-driven bow shock model is described in Figure 1.14 that shows a strong supersonic jet propagating in the surrounding interstellar medium, and the interaction between the jet and the ambient medium creating a thin outflow around the jet. Ahead of the jet, two shocks are also created: a jet shock (or termination shock) and a bow shock (or ambient shock). The impacted gas in between the shocks has a high pressure and is ejected out, thus creating an outflow cavity around the jet. The properties of the jet-driven bow shock model are detailed in Arce et al. (2007) and Gusdorf (2008).
**Figure 1.14:** Jet-driven bow shock configuration (Gusdorf, 2008).

**Figure 1.15:** Stellar wind-driven bow shock configuration (credit: N. Cox, KU Leuven).
1.4.2 Stellar wind-driven bow shock configuration

The stellar wind-driven bow shock model is described in Figure 1.15. Basically, the physical process is similar to the case of the jet-driven bow shock model. The freely supersonic stellar wind sweeps up the surrounding interstellar materials, causing the development of an astrosphere. At the inner edge of the astrosphere, the free flowing stellar wind switches from supersonic to subsonic through the wind shock (or termination shock). The wind material in the astropause is separated from the interstellar matter by a contact discontinuity, where turbulent features form due to shear forces and density differences between the two fluids. If the speed of the star relative to the ambient medium is supersonic, a bow shock (or ambient shock) is formed at the outer edge of the astropause.

1.5 Outline of the thesis

The structure of this thesis follows the delineation of the bow shock model in section 1.4. It consists of three parts. First, we build a bow shock model with a three dimensional morphology characterizing the shocked ambient material in the ISM, and we compare it to observations. Second, we study the stellar wind-driven termination shock. From an observational point of view, both jets and stellar winds create a bright termination shock which can be studied, but the launch mechanism of the jet is unclear and debatable, while the mechanisms and initial conditions that generate the wind are well studied (e.g., De Greve et al. 1997, Le Bertre et al. 1999, Gail and Sedlmayr 2013) and the outcomes match well to observations. Furthermore, we are collaborating with observers who have studied stellar winds, such as Le Bertre and Gérard (2004), Matthews et al. (2013), and Hoai et al. (2017), so we focus on winds rather than on jets. Third, we develop a spherical termination shock model, which physically and chemically couples the freely expanding stellar wind model (described in the second part) and the surrounding ISM.
Chapter 2

BOW SHOCKS

2.1 Molecular hydrogen: one of the best shock tracers

Molecular hydrogen H$_2$, the most abundant molecule in the universe, naturally exists in shocked regions. Since molecular hydrogen is homonuclear, it has no dipole moment and the rovibrational transitions only occur by electric quadrupole radiation ($\Delta J = 0, \pm 2$). No dipole moment leads to the weakness of the quadrupole transitions. Consequently, the first observable rotational transition ($J=2$) state lies at 509 K (28.2 $\mu$m) above the ground state, while the first vibrational transition ($v=1$) approximately lies at 6330 K (2.2 $\mu$m) above the ground state. The full rovibrational levels of H$_2$ used in this thesis are given in Appendix F.

Molecular hydrogen is a particularly important tracer, the mass fraction of which is important enough to determine the density of the gas. H$_2$ is one of the necessary element in order to help define the chemical state because it is at the origin of almost all chemical reaction chains that produce other molecules. In shocked regions, the temperature can rise up quickly and generate excitation both for rotational and vibrational levels as mentioned above. This makes H$_2$ a major coolant for the shocked gas. The strong emission of rovibrational lines, therefore, is a good tracer for the shock structure. In addition, because of rapid cooling, molecular hydrogen can be complemented by the excitation of other molecules such as CO, SiO, etc that have lower energy levels. As an example, Figure 2.1 is the BHR71 outflow composed of several data sets (Giannini et al., 2004). The structure of the outflow is mapped by CO on the left hand side and by H$_2$ on the right hand side. This figure visually indicates that CO and H$_2$ clearly probe the entire structure of the whole BHR71 outflow.
2.2 Excitation diagram

H$_2$ is one of the main tracers in shocked regions. In the following, we explain how to use it to deduce information on shocked regions. One effective way is to study the integrated intensity of rovibrational transitions to provide a good visualization of the physical conditions of the medium. This tool is known as the excitation diagram. The latter is a way to visualize the molecular hydrogen excitation state, by showing the logarithm of the column density of the excited rovibrational levels, divided by their statistical weight ($lnN_{v,j}/g_{v,j}$ with $N_{v,j}$ in cm$^{-2}$) against their excitation energy $E_{v,j}(K)$. Here, $vJ$ denotes the excited rovibrational levels and the statistical weight $g_{v,j} = I_s(2J + 1)$, where the nuclear spin statistical weight $I_s$ equals 1 (even rotational level $J$), and 3 (odd rotational level $J$).
The column density $N_{vJ}$ of a rovibrational level of H$_2$ is deduced from its line intensity $I_{vJ}$ through the spontaneous probability of deexcitation given by the Einstein coefficient $A_{vJ}$. If one assumes that a given line of H$_2$ emission is optically thin (which is usually the case given the very small values of $A_{vJ}$) the column density is then calculated by

$$N_{vJ} = \frac{4\pi \lambda_{vJ}}{hc} \frac{\lambda_{vJ}}{A_{vJ}} I_{vJ}$$

(2.1)

where $\lambda_{vJ}$ is the central wavelength of the line transition, $h = 6.626 \times 10^{-27}$ erg s is the Planck constant and $c = 2.998 \times 10^{10}$ cm s$^{-1}$ is the speed of light in vacuum. If the gas is thermally excited at temperature $T_{ex}$, the column density $N_{vJ}$ is proportional to the product between the statistical weight $g_{vJ}$ and the Boltzmann factor $e^{-\frac{E_{vJ}}{kT_{ex}}}$. If $T_{ex}$ is constant, ln$N_{vJ}/g_{vJ}$ and $E_{vJ}$ should be proportional with a slope equal to $T_{ex}^{-1}$. Therefore, this diagram allows us to roughly estimate the excitation temperature. In the situation of local thermal equilibrium, the excitation temperature $T_{ex}$ is equal to the gas temperature. Hereafter, we introduce how to use the H$_2$ excitation diagram to interpret observations.

### 2.3 Single shock model to interpret observations

H$_2$ emissions from pure shocked regions are the most interesting targets to study shock properties and to test shock models. Some shocks have been studied extensively, such as in the Orion Molecular Cloud - Peak1 (hereafter OMC-1 Peak1) (Rosenthal et al., 2000) (the brightest source of H$_2$ emission in the sky) and the BHR71 outflows (Gusdorf et al., 2015).

H$_2$ emission from the OMC-1 Peak1 is suggested to arise from shocks (Gautier et al. 1976, Brand et al. 1989). Over decades, single shock models have been investigated to answer the question of the physical nature of shocks, and the calculated excitation diagram has been widely used to fit to the observable shocks. However, Rosenthal et al. (2000) came to the conclusion that such models cannot fit the low and high excitation population levels simultaneously as shown in Figure 2.2. A combination of two single planar C-shocks (Kaufman and Neufeld, 1996) provides a good fit of the low excitation population levels corresponding to $v = 0$, $J = 3$ to 9, while it overestimates populations of higher levels. On the contrary, a single planar J-shock model (Brand et al., 1988) can match the medium and high excitation population levels, although it overestimates the population of lower levels. To conclude, no single stationary planar shock model can reproduce the observed H$_2$ level populations for the OMC-1 Peak1. Hence, a combination of at least two different shock models, one for the low excitation level populations and one for the higher excitation levels, may be required.
Le Bourlot et al. (2002) indicate that a two-component shock model including two planar shocks with different speeds, magnetized media and initial abundances of H can match well the observed H$_2$ from the OMC-1 Peak1 extending up to the rotational level $v = 0$, $J = 27$, which corresponds to an excitation energy of 42515 K (Figure 2.3). Specifically, the model with $v_s = 40$ km s$^{-1}$, $B_0 = 400$ μG, $n(H)/n(H_2) = 7.4 \times 10^{-4}$ fits well the lower excitation level populations $v = 0$, $J < 7$ and the higher level populations are in good agreement with the model characterized by $v_s = 60$ km s$^{-1}$, $B_0 = 100$ μG, $n(H)/n(H_2) = 0.5$. Despite the good fit, the origin of the difference between the two compounded shocks and why they should be linked remain unclear, as well as the properties of the ambient gas. Furthermore, the retrieved pre-shock density ($10^4$ cm$^{-3}$), corresponding to the best fit is lower by 2 orders of magnitude than the value ($\sim 10^6$ cm$^{-3}$) derived by (Draine and Roberge 1982, White et al. 1986, Brand et al. 1988, Hollenbach and McKee 1989, Kaufman and Neufeld 1996, Kristensen et al. 2008).

Can a non-stationary planar shock model match better the observations? To constrain the physical conditions of the shocked gas from the BHR71 outflow, Gusdorf et al. (2015) calculate the pure low rotational H$_2$ excitation diagram for 1200 models (Flower et al., 2003a), comprising both stationary shocks and non-stationary shocks and then they compare with diagram observed from the outflow. These authors figured out that the best fit is a non-stationary shock, and they estimated its age (Figure 2.4). However, the best diagram is different from that of the observed diagram: it falls down and crosses the observed one. That means that the non-stationary planar model overestimates the excited
H$_2$ column densities of the BHR71 outflow for levels at excitation energy less than that of the intersection point, otherwise it underestimates for the rest.

### 2.4 Bow shock models to observations

To go beyond the discussion in section 2.3, it is fair to examine more complex shock models with a higher number of spatial dimensions. One solution is to run 2D or 3D numerical simulations, but they have been so far limited to single-fluid "jump" bow shocks, J-type (e.g., Suttner et al. 1997, Raga et al. 2002). Up to now multidimensional bow shocks with "continuous" C-type shocks, where ion-neutral decoupling occurs in a magnetic precursor (Draine and McKee, 1993), have not been modeled. However, orthogonal and oblique planar shocks have been treated in simulations by Mac Low et al. (1995), Toth (1995), and Stone (1997). Such a situation is encountered in the bow shock whenever the entrance speed drops below the magnetosonic speed in the charged fluid. To address this case, one can predict H$_2$ emission from bow shocks by prescribing a bow shape and treat each surface element as an independent 1D plane-parallel J-type or C-type shock, assuming that the emission zone remains small with respect to the local curvature. This approach was first proposed by Smith and Brand (1990a) and Smith et al. (1991a) who used simplified equations only for the 1D C-shock structure and cooling. In the same way, Smith et al. (1991b) reproduced the line profile of H$_2$ emission from OMC-1 Peak1, observed by Moorhouse et al. (1990) (Figure 2.5). However, this model requires an extremely high
magnetic field (>50 mG), when independent measurements show that it should range from 3 mG (Norris, 1984) to 10 mG (Chrysostomou et al., 1994) in the same region.

The validity of this approach was actually recently investigated by Kristensen et al. (2008) and Gustafsson et al. (2010) who used refined 1D steady-state shock models from Flower and Pineau des Forêts (2003) that solve the full set of magneto-hydrodynamical equations with non-equilibrium chemistry, ionization, and cooling.

Kristensen et al. (2008) studied high angular resolution H$_2$ images of a bow shock in the Orion BN-KL outflow region, performing several 1D cuts orthogonal to the bow trace in the plane of the sky. They fitted each cut separately with 1D steady shock models. They found that the resolved width, combined with the peak brightness required C-shocks, and that the variation of the fitted shock velocity and the transverse magnetic field along the bow surface was consistent with a steady bow shock propagating in a uniform medium. This result provided some validation for the "local 1D-shock approximation" when modeling H$_2$ emission in bow shocks, at least for this parameter regime. Following this idea, Gustafsson et al. (2010) built 3D stationary bow shock models by stitching together 1D
Figure 2.5: Bow shock models fits to OMC-1 Peak1 shock. The points denote the observational data, the solid line is the best fit (Smith et al., 1991b).

shock models. Then they projected them to produce maps of the H₂ emission in several lines that they compared to observations. They obtained better results than Kristensen et al. (2008) thanks to the ability of the 3D model to account both for the inclination of the shock surface, with respect to the line of sight, and the multiple shocks included in the depth of their 1D cuts. The width of the emission maps was better reproduced. The best fit density, bow shock inclination and ambient magnetic field all agreed with independent constraints.

2.5 Power-law statistical equilibrium assumption

Neufeld and Yuan (2008) (hereafter NY08) and Neufeld et al. (2009, 2014) came up with a simple model assuming statistical equilibrium for a power-law temperature distribution $T^{-b}dT$. The corresponding column density of gas at temperature between T and dT is

$$dN = aT^{-b}dT$$

(2.2)

with $a, b$ adjustable parameters. The temperature ranges between 100 K and 4000 K. This assumption turns out to be very effective at reproducing the pure rotational lines of H₂
To interpret their results, these authors proposed the effect of the three-dimensional bow shock geometry. Owing to an accumulation of the bow shock surface, the mass of material crossing the working surface $dA$ with velocity from $v$ to $v + dv$ perpendicular to the shock surface should be

$$dM \propto N(H_2)dA. \quad (2.3)$$

For a parabolic shape of shock, Smith and Brand (1990b) showed that $dA \propto v^{-4}$ ($\forall v < v_{bow}$, terminal velocity at the head of bow shock). Neufeld et al. (2006) found that the column density of $H_2$ was proportional to velocity as $v^{-0.75}$ and the velocity was related to temperature as $T^{1/1.35}$ for a single C-shock. Combining all of those relations, Equation 2.3 yields

$$dM \propto v^{-0.75}v^{-4}dv \propto T^{-3.77}dT. \quad (2.4)$$

Therefore, in the specific case of a parabolic shock shape, the power-index is expected to be $b=3.77$.

### 2.6 Aims and outline

Several models have been designed to reproduce the properties of bow shocks, most of them are one-dimensional (see section 2.3). In order to better match the observations, we will investigate shock models with more complex geometries. Based on the method of Kristensen et al. (2008) and Gustafsson et al. (2010), we have built a 3D shock model made of 1D shock models stitched together. To extend the scope of the works of Gustafsson et al. (2010), we provide a general way to encode the 3D geometry of a bow-shock as a distribution of shock models. In addition, we consider the effect of young shock ages, where the shock is not stationary, and we investigate thoroughly the impact of various shock characteristics on the excitation diagram and line profiles integrated over the bow of the molecular hydrogen. Then we compare our 3D bow shock model with observations. The best fit provides us with constraints on some physical parameters of the bow shock.

We structure this part as below:

- Chapter 4: we recall the principles of the 1D Paris-Durham shock model (Flower and Pineau des Forêts 2015a, Flower et al. 2003a) and we introduce the physical and chemical input parameters.
- Chapter 5: we describe how to build the 3D bow shock by stitching several 1D Paris-Durham shock models.
Figure 2.6: Best fitting of the power-law statistical equilibrium assumption. Diamonds indicate the observed values, and the solid lines are the best fitting procedure by the power-law statistical equilibrium assumption from Neufeld and Yuan (2008) (Equation 2.2). In this studies, the values of the power-index is in the range 2.3-3.3 (Neufeld et al., 2009).

- Chapter 6: we describe the procedure to fit the 3D bow shock model to the observations.
- Chapter 7: we summarize the achievements of our model and we sketch the prospects for future improvements and applications.

Chapters 5 and 6 follow very closely Tram et al. (2018), with only a few additions.
Chapter 3

WIND AND TERMINATION SHOCKS

Beside bow shocks occurring in the ambient material (chapter 2), a termination shock also forms at the head of jet outflows and in the bulk of the stellar wind surrounding the stars. As mentioned in section 1.5, our study is focused on the termination shocks around Asymptotic Giant Branch (AGB) stars. In this chapter, we introduce the characters of AGB star winds and their interaction with the ISM.

3.1 Stellar winds from AGB stars

As described earlier, low- and intermediate-mass stars \((1 M_\odot \leq M_\ast \leq 8 M_\odot)\) reach the AGB phase, which is the last stage of their evolution before they become a white dwarf. During this phase, the star has lost most of its material throughout mass loss mechanisms. Material can be lost only when its flow exceeds the star’s gravity. In the absence of a pressure gradient, for example when it has accelerated and its speed exceeded the escape speed, there is no turning back.

While the flow remains subsonic, several mechanisms for initiating winds close to the star have been suggested: gradient of gas pressure (thermal wind), acceleration through waves (sound wave, Alfvén wave), or pulsations. Pulsations are currently the dominant paradigm (e.g., Hoefner and Dorfi 1997, Willson 2000) to lift up materials from the stellar surface into cooler regions (dust shell acceleration zone in Figure 3.1), where molecules and dust grains can form. The latter scatter and absorb the stellar photons, which leads to a net force pushing them away from the star. Then they move through the gas and transfer momentum to gas molecules due to collisions. Tielens (1983) and Krueger et al. (1994) found that the dust grains always move with their equilibrium drift velocity with respect to the gas, which is of the order of the isothermal sound speed or higher. Therefore, while
the grains are not position-coupled to the gas, they are momentum-coupled to the gas. Those collisions produce a drag force (Gilman 1972), which acts as an additional force sufficient for the gas to overcome the gravitational well of the star. In this case, the wind is called a *dust-driven wind* or a *radiation-driven wind*.

### 3.2 Circumstellar envelopes around AGB stars

Mass-loss from stars builds up an expanding circumstellar envelope (CSE) around the star, containing dust and gas. The mass-loss mechanism affects the geometry of the CSE. Most of the time, the CSE is not observed as a spherical symmetric or a homogeneous envelope, which hints that the mass-loss is not an isotropic process.

Circumstellar envelopes of AGB stars can be considered as the most significant chemical laboratories in the universe (Table 3.1 and Figure 3.2). The effective temperature of those stars is usually low \( T_e \approx 2000 \, \text{K} - 3500 \, \text{K} \) (comes from Infrared observations), and the timescale of the mass-loss is long, so that molecules and dust can form in the envelope through chemical and physical processes. Then they are blown into the interstellar medium. This material can dominate about 80% of the ISM by mass (Jorgensen, 1994).


### Table 3.1: Chemical species observed by the Submillimeter Telescope (SMT) of the Arizona Radio Observatory (ARO) toward IRC +10216 and VY CMa in Figure 3.2 (Tenenbaum et al., 2010).

| Carbon-rich star | Oxygen-rich star |
|------------------|------------------|
| CO               | CO               |
| SiO              | CCH              |
| SiS              | NaCN             |
| CS               | l-C$_3$H         |
| CN               | c-C$_3$H         |
| HCN              | H$_2$C0          |
| HNC              | H$_2$CS          |
| NaCl             | HC$_3$N          |
| PN               | C$_2$H           |
| HCO$_3$          | CH$_3$CN         |
| PH$_3$           | CH$_3$CCH        |
| CH$_2$NH         | Unidentified     |
| CP               | AIO              |
| SiC              | AIOH             |
| AlCl             | SO               |
| KCl              | H$_2$O           |
| AlF              | SiO              |
| SiN              | H$_2$S           |
| HCP              | Unidentified     |

#### 3.2.1 Circumstellar gas molecules

The origin of the circumstellar gas lies inside the stellar core through its evolution stages (see section 1.3). Briefly, $^{12}$C, $^{14}$N and $^{16}$O are produced through the fusion of helium and alpha process. The dredged-up processes then bring those nuclear products up to the stellar surface.

Most of the known circumstellar gas molecules are detected in carbon-rich stars (mostly only in IRC +10216). Observations toward IRC +10216, have detected about 71 chemical components in its CSE (e.g., Cernicharo et al. 2000, He et al. 2008). However, despite speculations that the oxygen-rich CSEs are less chemically diverse (Olofsson, 2005), recent observations of VY CMa star (Tenenbaum et al., 2010) demonstrate that oxygen-rich stars are also chemically complex: about 32 different chemical species have been identified in their CSEs. Figure 3.2 shows the spectral line survey of the Submillimeter Telescope (SMT) of the Arizona Radio Observatory (ARO) toward the carbon-rich star (IRC +10216) and oxygen-rich star (VY CMa). The names of detected species are listed in Table 3.1.
FIGURE 3.2: Chemical species observed by the Submillimeter Telescope (SMT) of the Arizona Radio Observatory (ARO) toward IRC +10216 and CY CMa. (Upper panel) Complete spectra of the ARO SMT survey in 214.5-285 GHz. (Lower panel) Detailed 1 GHz selection centered at 267 GHz of the survey (Tenenbaum et al., 2010).
Chemical models have been created to explain the formation mechanisms of those species in order to understand the chemical processes in the ISM (e.g., Willacy and Cherchneff 1998, Agúndez and Cernicharo 2006, Cherchneff 2006, Decin et al. 2010, Li et al. 2016). Based on these studies, the authors demonstrate that the temperature and density in the inner envelope ($r \lesssim 5R_\odot$), although high, does not satisfy the thermal equilibrium conditions as a result of shock propagation, and chemistry is also out of equilibrium. "In any case, molecular abundances derived from TE calculations should not be used in the interpretation of observational data which are not of the photosphere" (Cherchneff, 2006).

The chemistry strongly depends on the radius and remarkably varies through the circumstellar envelope as indicated in Figure 3.3. In the inner region, the inner shocks trigger the formation of molecules and dust. Those molecules are called "parent" abundances. As molecules flow outward to the outer envelope, the "parent" abundances freeze out, and photons, cosmic rays and interstellar radiation field initiate new types of chemical processes, such as ion-molecule, photo-dissociation/ionization reactions that create new molecules (e.g., Millar et al. 2000, Decin et al. 2010, Li et al. 2016). Those newly formed molecules are called "daughter". Beyond $\sim 1000$ AU, the photo-dissociation by the interstellar radiation field is so strong that the gas molecules cannot subsist (Figure 3.1). The dissociation radius is different for each molecule depending on the efficiency of its screening to photo-dissociation, and it also depends on the mass-loss rate and expansion velocity.
3.2.2 Circumstellar dust

Beside molecules, the circumstellar envelope is made of a various circumstellar dust particles and is identified by their properties. The dust is thought to be formed by a mechanism of gas-phase molecule condensation (Kwok, 2004) during the expansion of the CSE (Figure 3.1). The conditions for dust formation are low temperature (to allow for condensation) and high density (to allow for sufficient interaction rate). Typical condensation radii of dust range from 5 to 10 stellar radii, corresponding to a temperature varying from 1000 K down to 600 K and a total number density varying from $10^{10}$ to $10^{8}$ cm$^{-3}$.

Since oxygen and silicon are amongst the most abundant molecules in the universe, silicates are believed to be reasonably common in the CSE of AGB stars. Most of the identified silicates are amorphous, which satisfies the expectation of rapid formation of amorphous material in gas-phase environment. Some materials, in particular, have high condensation temperatures and can condense at $\sim$2 photospheric radii and act like seed particles for further grain growth (Lorenz-Martins and Pompeia, 2000).

Dust grains are classified by their spectral features and they correspond to a special kind of envelope properties. Amorphous silicates, identified at 9.7 and 18 $\mu$m, have been detected in more than 4000 oxygen-rich stars (Kwok et al., 1997), thus they are considered as a major feature of oxygen-rich stars. In addition, Jaeger et al. (1998) found clear evidence for the existence of crystalline silicates in the spectra measured by the Short Wavelength Spectrometer (SWS) of the Infrared Space Observatory (ISO). The crystalline silicates are found in two forms: olivine (Mg$_{2y}$Fe$_{2-2y}$SiO$_4$) and pyroxene (Mg$_{x}$Fe$_{1-x}$SiO$_3$) (Dorschner et al., 1995). Jaeger et al. (1998) also point out that crystalline silicate in the CSE of the oxygen-rich stars is magnesium-rich, which means that $x$, $y$ are close to unity. However, the abundance of the crystalline form is smaller than that of the amorphous form (Kwok, 2004).

Silicate carbide, which has a 11.3 $\mu$m-feature is the most common dust grain condensed in the CSE of carbon-rich stars. It has been detected in over 700 carbon-rich stars (Kwok et al., 1997). In more evolved carbon-stars (the abundance of C is much larger than O), the silicon carbide, however, becomes weaker and the amorphous carbon increasingly dominates (Kwok, 2004). In addition to silicon carbide and amorphous carbon, the Infrared Astronomical Satellite (IRAS) observations with Low Resolution Spectrometer (LRS) toward carbon-rich stars find an evidence for 21 $\mu$m emission (Kwok et al., 1989). The solid-state structure of this strong emission is uncertain. Some possible candidates have been proposed, such as large polycyclic hydrocarbon (PAH) (> 100 C atoms) cluster, hydrogenated amorphous carbon (HAC) grain (Buss et al., 1990), nanodiamonds (Hill et al., 1998), etc.
Dust grains are opaque, and scatter the stellar light. Therefore, the size of the condensation dust shell can be determined by: (i) IR emission since stellar photons heat up grains, which then produce IR radiation by cooling (Figure 3.4, left panel), (ii) the scattered light (Figure 3.4, central panel), and (iii) polarized light since light becomes polarized when it is scattered by grain particles (Figure 3.4, right panel).

### 3.3 Interaction with the ISM

As it reaches the ISM, the stellar wind interacts with it and sweeps up the surrounding materials. Thanks to infrared observations from Herschel, Cox et al. (2012) showed different kinds of morphology of the interaction modes. The hydrodynamic mechanisms are well studied (e.g., Cox et al. 2012, Villaver et al. 2012).

As described in section 2.1, hydrogen is the best tracer for the interaction between the stellar wind and the ISM. Studies of HI 21 cm emission (e.g., Gérard and Le Bertre 2006, Gérard et al. 2011, Libert et al. 2007, 2008, 2010a,b, Matthews and Reid 2007, Matthews et al. 2008, 2011, 2013) conclude that neutral hydrogen is a good tracer of the extended CSEs. Since in the absence of strong UV, hydrogen is not easily ionized, its emission can therefore trace the very large scales of CSEs, larger than CO, which is easily dissociated by the interstellar radiation field (ISRF) at a distance of $\sim 10^{17}$ cm from the stars.

Although part of the hydrogen is locked into non-linear molecules, such as H$_2$O, most of it is in either atomic or molecular form (Gérard and Le Bertre, 2003). The fractional ratio between atomic and molecular hydrogen in the CSEs has been discussed by Glassgold
and Huggins (1983). For "high" stellar effective temperature ($T_{eff} > 2500$ K), hydrogen should be mainly in atomic form. In contrast, for stars with "low" effective temperature ($T_{eff} \leq 2500$ K) it should be in molecular form in the upper atmosphere and in the inner CSE. This hypothesis seems to be confirmed by the detection of a 21 cm emission line in CSEs of "hot" AGB stars, such as Mira (Bowers and Knapp, 1988), RS CnC (Gérard and Le Bertre, 2003), EP Aqr (Le Bertre and Gérard, 2004), Xher (Gardan et al. 2006, Matthews et al. 2011), Y CVn (Le Bertre and Gérard, 2004), and the detection of FUV emission from the "cold" AGB star IRC +10216 (Sahai and Chronopoulou, 2010), which is believed to trace the interaction between molecular hydrogen and electrons (see subsection 1.3.2). However, Matthews et al. (2015) recently discovered a thin shell of HI, the total mass of which is less than 1% compared with the total predicted mass of the CSE of the "low" stellar effective temperature (IRC +10216). These authors suspect that this small amount of HI results from the photo-dissociation of H$_2$ by the ISRF as suggested by Glassgold and Huggins (1983)'s model.

Despite all the above, the physical-chemical mechanisms that transfer hydrogen from the stellar surface into the inner part of the CSEs, and then into its outer part, as well as its conversion processes, have not been well studied.

Some of the observed HI lines have been successfully interpreted by simple hydrodynamic models (Libert et al. 2007, Hoai et al. 2015, 2017). Their "standard" stationary model is described in Figure 3.6. The free wind expansion takes place at $R_e < r < r_1$. The termination shock is located at $r_1$. The bow-shock is located at $r_2$. The wind and ambient materials are separated at $r_f$. For the region of freely expanding wind, the temperature and hydrogen number density are assumed to depend on radius as a power-law, $T \sim r^{-0.5}$, $n_H \sim r^{-1.5}$.
and \( n_H \sim r^{-2} \). For the terminal shock region \( (r_1 \leq r \leq r_f) \), the temperature, the velocity and the density are derived by solving the set of fluid dynamic equations for ideal gases, adopting the upstream conditions: velocity is obtained from observations, density is calculated from the mass-loss rate, and temperature is equal to \( T_0 = 20 \) K (Libert et al., 2007). For the external region \( (r_f < r < r_2) \), the density is again assumed to be \( r^{-2} \), and temperature is constant.

This simplified model that only accounts for the main hydrodynamic processes already nicely reproduces the spectrum of HI, such as for Y CVn (Figure 3.5, left panel). In this work we will attempt to improve the dynamical treatment by adding the coupling between the dust grains and gas and by including heating and cooling processes as done in steady-state wind models (Justtanont et al. 1994, Winters et al. 1994, Decin et al. 2006). Finally, we will also include time-dependent chemistry, in a hope to predict the fractional abundance of HI in the CSE.

In addition, Villaver et al. (2002) carefully studied the time dependent hydrodynamics of the circumstellar envelope. These authors took into account the thermal pulsation effect and the influence of the external ISM. Hoai et al. (2015) use this model to reproduce the Y CVn HI line shape. They compute the model at three different epochs corresponding to the first two thermal pulses and to the end of the last thermal pulse. However, the gas temperature in the CSE remains large (> 5000 K), which makes thermal broadening dominating the line profile. Consequently, the full-width at half-maximum (FWHM) is larger than the observed one (Figure 3.5, right panel).
3.4 Aims and outline

During the AGB phase, dredge-up processes mix the nuclear products deep inside the core up to the surface, and a mass-loss mechanism ejects them into the ambient medium. AGB stars lose most of their material through stellar winds, which eventually make up the circumstellar material around the star. The mechanisms that launch the material from the stellar surface into the CSE are well studied (see section 3.1). Since the temperature dramatically cools down further away from the stellar surface, the parent molecules and dust form (see section 3.2). Then the dust absorbs stellar radiation, and it couples and transfers momentum to the gas. This impact acts like an acceleration processes which pushes the gas away from star. The gas flow thus crosses the "critical point" where its speed exceeds the thermal sound speed, and the wind becomes supersonic. This supersonic wind eventually interacts with the ISM.

The whole collection of processes which take place in the CSE makes it look like a chemical factory. Among chemical species, hydrogen turns up as an important tool for tracing the large scale of the CSE (see section 3.3). The hydrodynamical models, whose outcomes match well the existing HI observations, could be improved to interpret better the hydrogen atomic and molecular fractions. Hence, in this part, we aim at studying the hydrogen chemistry in the CSE.

- Chapter 8: from the Paris-Durham shock code, we re-create a stationary hydrodynamic wind model in 1D spherical geometry. Although the preferred driving mechanism in the sub-sonic region is thermal pulsations, we assume that pressure gradient that lifts material up from the stellar surface. We also introduce a chemical network, which is coupled with the hydrodynamic model above.

- Chapter 9: we calculate the line profiles of the atomic hydrogen, including the termination shock, and compare them to observations.

- Chapter 10: we discuss the results and future prospects of our model.
Part II

BOW SHOCK MODEL
Chapter 4

1D-SHOCK MODEL: PARIS-DURHAM

The Paris-Durham\textsuperscript{1} shock code is born from a long term collaboration between David Flower in Durham and G. Pineau des Forêts in Paris. The first version of the Paris-Durham code was introduced by Flower et al. (1985) with the main objective of simulating 1D steady-state shocks propagating through the interstellar medium. That version included gas-phase chemical processes, studied by Flower and Pineau des Forêts in a series of articles published from 1985 to 1989. The solid-phase chemical processes were included in the next series of papers (e.g., Flower and Pineau des Forêts 1994, 1995, Pineau des Forêts and Flower 1996). As shown by Lesaffre et al. (2004a,b), the Paris Durham shock code can also compute approximations to 1D non steady-state magnetohydrodynamical shocks by glueing together pieces of steady-state models. Over the time, motivated by spectroscopy data acquired from satellites (ISO, Herschel, and Spitzer), the code has been improved to study the intensities of the molecular lines in sub-mm and in the infrared. In its recent state-of-the-art version, the Paris-Durham code is mainly written in FORTRAN 90, except for a few routines that are coded in FORTRAN 77. It uses the DVODE algorithm\textsuperscript{2} to solve the ODE equations. Flower and Pineau des Forêts (2015a) presents the official up to date version.

4.1 Magnetohydrodynamic shock wave

Magnetohydrodynamic (MHD) shock waves have been well studied in astrophysics because the astrophysical gas is usually magnetized, with a magnetic pressure comparable

\textsuperscript{1}Also known as the Durham-Paris shock code on the other side of the Channel

\textsuperscript{2}https://computation.llnl.gov/casc/odepack/
to the turbulent pressure of the gas. That kind of wave is very common in the interplanetary medium, the interstellar medium and in the star formation regions. The ionization fraction of the gas is very important to the study of shock waves, because the magnetic field directly interacts with the ionized gas and indirectly with the neutral gas via the collisions between the charged particles and the neutral particles. If the gas is ionized enough in a shock wave, the coupling between the charged particles and the neutral particles is strong so that the gas behaves like a single-fluid. Conversely, if the gas is weakly ionized, the collisions occur and the gas behaves like a multi-fluid. The principles of MHD shock waves and the main differences between those fluids are discussed below.

4.1.1 Set of conservation equations

In general, the dynamical state of the gas is identified by the number density $n$, the mass density $\rho$, the velocity $v$ and the temperature $T$, which are calculated from a set of conservation equations of number density, mass density, momentum and energy of neutral and charged fluids. The subscript "n" is used for the neutral particles and "i" for the ionized particles. In the shock plane, let us denote: (1) $z$ an independent variable, which defines the positive coordinate of the gas flow with respect to an arbitrary reference point in the pre-shock gas, (2) $t$ the corresponding traveling time of the flow, and (3) $B$ the transverse magnetic field perpendicular to the flow. With this simplified hypothesis, we can ignore the inherent complication of the oblique model, in which the magnetic field and the shock propagation creates an angle different from 90° with respect to the $z$-direction.

The conservation equation for the number density of neutral particles is

$$\frac{\partial n_n}{\partial t} + \frac{\partial}{\partial z}(n_n v_n) = N_n.$$  \hspace{1cm} (4.1)

where $N_n$ is the number of neutral particles created per unit volume and time. A corresponding equation holds for the charged particles

$$\frac{\partial n_i}{\partial t} + \frac{\partial}{\partial z}(n_i v_i) = N_i.$$  \hspace{1cm} (4.2)

The mass conservation of neutral fluid is written by

$$\frac{\partial \rho_n}{\partial t} + \frac{\partial}{\partial z}(\rho_n v_n) = S_n.$$  \hspace{1cm} (4.3)
where \( S_n \) is the neutral mass change due to chemical reactions. The corresponding equation for the positive charged fluid is

\[
\frac{\partial \rho_i}{\partial t} + \frac{\partial}{\partial z}(\rho_i v_i) = -S_n. \tag{4.4}
\]

The momentum of the fluid is also conserved. For the neutral fluid, the equation of momentum conservation is

\[
\frac{\partial}{\partial t}(\rho_n v_n) + \frac{\partial}{\partial z}\left(\rho_n v_n^2 + n_n k_B T_n + \pi_v\right) = A_n \tag{4.5}
\]

where \( A_n \) denotes the change of momentum of the neutral fluid per unit volume and time. \( k_B \) is the Boltzmann constant and \( n_n k_B T_n \) is the thermal pressure of the neutral fluid. \( \pi_v = \rho_n \lambda_0 c_0 \frac{\partial n}{\partial z} \) is a viscous pressure built with a constant viscous length and velocity \( \lambda_0 = 3 \times 10^{14} \) cm and \( c_0 = 1 \) km s\(^{-1}\). The viscous term hence diffuses momentum over a typical length scale \( \lambda_0 \) at a dispersion speed \( c_0 \). It is switched on when we want to trigger a viscous discontinuity (J-type, see subsubsection 4.1.3.2) in the flow, and it is switched off whenever \( \pi_v \) gets back below one part per million of the thermal pressure. In effect, viscosity dissipates ordered kinetic energy into heat.

If the magnetic field is accounted for, it acts directly onto the charged fluids and indirectly onto the neutral fluid through collisions and it adds a magnetic pressure term \( B^2/8\pi \) to the equation of momentum conservation. Thereby, the equation of momentum conservation for ion-electron fluid is

\[
\frac{\partial}{\partial t}(\rho_i v_i) + \frac{\partial}{\partial z}\left(\rho_i v_i^2 + n_i k_B (T_i + T_e) + \frac{B^2}{8\pi}\right) = -A_n. \tag{4.6}
\]

The equation of conservation of energy for the neutral fluid yields

\[
\frac{\partial}{\partial t}\left(\frac{1}{2}\rho_n v_n^2 + \epsilon\right) + \frac{\partial}{\partial z}\left(\frac{1}{2}\rho_n v_n^3 + \frac{\gamma}{\gamma - 1} v_n n_n k_B T_n + v_n \pi_v\right) = B_n \tag{4.7}
\]

where \( B_n \) is the change of energy of the neutral fluid per unit volume and time, \( \epsilon \) is the internal specific energy, and \( \gamma \) is the adiabatic index. For the ion-electron fluid, similarly, the magnetic field adds one more term \( B^2/4\pi \) due the magnetic energy flux:

\[
\frac{\partial}{\partial t}\left(\frac{1}{2}\rho_i v_i^2 + \epsilon\right) + \frac{\partial}{\partial z}\left[\frac{1}{2}\rho_i v_i^3 + \frac{\gamma}{\gamma - 1} v_i n_i k_B (T_i + T_e) + \frac{B^2 v_i}{4\pi}\right] = B_i + B_e. \tag{4.8}
\]
4.1.2 Source terms

The source terms $N$, $S$, $A$ and $B$ which appear on the right hand side of the equations of conservation respectively represent the rate of change in number density, mass, momentum and energy per unit volume of the neutral to charged fluids through irreversible micro-physics processes. These mechanisms in fact depend on the context being considered. In this section, we summarize some of the main source terms that may appear in interstellar molecular clouds. Further details can be found in Flower et al. (1985) and Flower and Pineau des Forêts (2015b).

4.1.2.1 Number and mass of particles source terms

If $\alpha$ is a particular atomic or molecular species, and $C_\alpha$ is the net production of species $\alpha$ per unit volume, the rates of change of the total number of neutral species and positive ion per unit volume are

$$N_n = \sum_{\alpha} C_\alpha \quad \text{ (neutral species)}$$

$$N_i = \sum_{\alpha} C_\alpha \quad \text{ (ionized species)}$$

The changing rate of neutral and positive ion mass are then

$$S_n = \sum_{\alpha} C_\alpha m_\alpha \quad \text{ (neutral species)}$$

$$S_i = \sum_{\alpha} C_\alpha m_\alpha \quad \text{ (ionized species)}$$

4.1.2.2 Momentum source terms

Let us denote $C_{\alpha\beta}$ the creation ($C_{\alpha\beta} > 0$) or the destruction ($C_{\alpha\beta} < 0$) rates of species $\alpha$ through the reaction $\beta$. Therefore,

$$C_\alpha = \sum_{\beta} C_{\alpha\beta} \quad \text{ (4.13)}$$
Through the ion-neutral reactions, the charged fluid transfers momentum to the neutral fluid at rate $A_{n}^{(1)}$

$$A_{n}^{(1)} = \sum_{(\text{neutral speci})} \sum_{\beta} C_{\alpha\beta} m_{\alpha} v_{\beta}(CM)$$  \hspace{1cm} (4.14)

where $v_{\beta}(CM)$ is the collision center-of-mass velocity defined as

$$v_{\beta}(CM) = \frac{m_{i} v_{i} + m_{n} v_{n}}{m_{i} + m_{n}}$$  \hspace{1cm} (4.15)

where $m_{i}$, $m_{n}$ are the mass of ions and neutral reactants, and $\beta$ is the dummy index for ion-neutral reactions with net rate $C_{\alpha\beta}$. Equation 4.14 indicates that species are created and destroyed at the center-of-mass collision velocity $v_{\beta}(CM)$.

Owing to elastic scattering on the ions, the neutral fluid gains momentum at a rate $A_{n}^{(2)}$

$$A_{n}^{(2)} = \frac{\rho_{n}\rho_{i}}{\mu_{n} + \mu_{i}} <\sigma v>_{in} (v_{i} - v_{n})$$  \hspace{1cm} (4.16)

where the rate coefficient is defined by

$$<\sigma v>_{in} = 2.41 e \left( \frac{\alpha_{n}}{\mu_{in}} \right)^{\frac{1}{2}}$$  \hspace{1cm} (4.17)

in unit of $\text{cm}^{3} \text{s}^{-1}$, with $\alpha_{n}$ the polarizability of the neutral fluid, $\mu$ the mean molecular weight and $\mu_{in} = \mu_{i}\mu_{n}/(\mu_{i} + \mu_{n})$ the reduced mass.

In the case of a dense cloud medium where the ionization degree of the gas is small, momentum transfer between the neutral fluid and the charged grains is important. The collision cross-section can be approximated by the grain cross-section $\pi a_{g}^{2}$, where $a_{g}$ is the grain radius, and the collision speed is close to the ion-neutral drift $|v_{i} - v_{n}|$. Hence, the rate of momentum transfer between the neutral fluid and the charged grains derives from Equation 4.16 with $\mu_{g} \gg \mu_{n}$ as

$$A_{n}^{(3)} = \rho_{n} n_{g} \pi a_{g}^{2} |v_{i} - v_{n}| (v_{i} - v_{n}).$$  \hspace{1cm} (4.18)

The total rate of change for the neutral fluid momentum is then the sum of momentum transfer from those processes $A_{n} = A_{n}^{(1)} + A_{n}^{(2)} + A_{n}^{(3)}$.

4.1.2.3 Energy source terms

The micro-physical processes along the shock also lead to energy exchanges between the charged and the neutral fluids, as well as between the charged grains and the neutral fluid.
Chemical reactions are responsible for part of the kinetic energy transfer from the charged to the neutral fluids. The exchange rate per unit volume through the chemical reactions $\beta$ is derived from Equation 4.14

$$B_n^{(1)} = \sum_{\text{neutral species}} \sum_{\beta} C_{\alpha\beta} \frac{1}{2} m_{\alpha} v_{\beta}^2 (CM).$$  \hspace{1cm} (4.19)

When an ion at temperature $T_i$ dissociatively recombines with an electron at temperature $T_e$ to form two neutral species, an amount of energy $3/2k_B(T_i + T_e)$ is transferred to the neutral fluid. On the contrary, when a neutral is photo-ionized, it loses an amount of heat $3/2k_B T_n$. The heat rate transfer to the neutral fluid per unit volume is then

$$B_n^{(2)} = \sum_{\text{neutral species}} \left[ \sum_{\beta (C_{\alpha\beta} > 0)} C_{\alpha\beta} \frac{3}{2} k_B (T_i + T_e) + \sum_{\beta (C_{\alpha\beta} < 0)} C_{\alpha\beta} \frac{3}{2} k_B T_n \right].$$  \hspace{1cm} (4.20)

The chemical reactions can also affect the thermal balance of the medium via the chemical energy released $\Delta E$. This heats the neutral fluid with a corresponding rate

$$B_n^{(3)} = \sum_{\text{neutral species}} \sum_{\beta} C_{\alpha\beta} \frac{M_{\beta} - m_{\alpha}}{M_{\beta}} \Delta_{\beta}$$  \hspace{1cm} (4.21)

where $M_{\beta}$ is the total mass of the products from reaction $\beta$ and $\Delta_{\beta}$ is the net chemical energy released by this reaction.

The elastic scattering of the neutral fluid on the ions results to a rate of heating for the neutral fluid as

$$B_n^{(4)} = \frac{\rho_n \rho_i}{\mu_n \mu_i} < \sigma v >_{\text{in}} \frac{2 \mu_n \mu_i}{(\mu_n + \mu_i)^2} \left[ \frac{3}{2} k_B (T_n + T_i) + \frac{1}{2} (v_i - v_n)(\mu_i v_i + \mu_n v_n) \right].$$  \hspace{1cm} (4.22)

The elastic scattering of the neutral fluid on the electrons results to the same rate of heating for the neutral fluid, except for the fact that $m_e \ll m_n$

$$B_n^{(5)} = \frac{\rho_n \rho_e}{\mu_n \mu_e} < \sigma v >_{\text{en}} \frac{2 \mu_e}{\mu_n} \left[ \frac{3}{2} k_B (T_n + T_e) + \frac{1}{2} (v_i - v_n)(\mu_i v_i + \mu_n v_n) \right]$$  \hspace{1cm} (4.23)

where the scattering cross section is

$$< \sigma v >_{\text{en}} = 10^{-15} \left( \frac{8 k_B T_e}{\pi m_e} \right)^\frac{1}{2}.$$  \hspace{1cm} (4.24)
The rate of energy transfer from the charged grains to the neutral fluid is derived from Equation 4.18

\[ B_n^{(6)} = \rho_n n_g \pi a_n^2 |v_i - v_n| (v_i - v_n) v_i \]  

(4.25)

The total rate of energetic change for the neutral fluid \( (B_n) \) is also the sum all of those processes \( B_n = B_n^{(1)} + B_n^{(2)} + B_n^{(3)} + B_n^{(4)} + B_n^{(5)} + B_n^{(6)} \). The total rate of energetic change for the ionized fluid \( (B_i) \) proceeds similarly to the neutral fluid.

The electron particles can transfer energy via three main processes: (1) dissociatively recombining with an ion, (2) scattering on ions and (3) through photo-ionization.

As described in Equation 4.20, when an electron at temperature \( T_e \) dissociatively recombines with an ion to create neutral species, it loses an amount of heat

\[ B_e^{(1)} = \sum_{\alpha} \sum_{\beta} C_{\alpha,\beta} \frac{3}{2} k_B T_e \]  

(4.26)

The heat can also be transferred between the fluid of electrons and the fluid of ions through collisions. The heating rate can be determined as

\[ B_e^{(2)} = \frac{4e^4}{\mu_i k_B T_e} \left( \frac{2\pi m_e}{k_B T_e} \right)^{\frac{1}{2}} \ln \Lambda \left( \frac{\rho_i}{\mu_i} \right)^2 k_B (T_i + T_e) \]  

(4.27)

where

\[ \Lambda = \frac{3}{2e^3} \left( \frac{k_B^3 T_e^3 \mu_i}{\pi \rho_i} \right)^{\frac{1}{2}}. \]  

(4.28)

The rate of heating through photo-ionization should be

\[ B_e^{(3)} = \sum_{\alpha} \delta E_\alpha \gamma_\alpha n_\alpha \]  

(4.29)

where \( \delta E_\alpha \) is the mean energy of the photo-electron created by the photo-ionization of the species \( \alpha \), with density \( n_\alpha \) and photo-ionization rate \( \gamma_\alpha \).

The total rate of energetic change for the electron fluid is \( B_e = B_e^{(1)} + B_e^{(2)} + B_e^{(3)} \).

In addition, the Paris-Durham code incorporates a wide range of cooling and heating processes relevant to the ISM. Lyman \( \alpha \) cooling is included as well as line excitation cooling from neutral atoms and ions: C, N, O, S, Si, C\(^+\), N\(^+\), O\(^+\), S\(^+\), Si\(^+\), Fe\(^+\). We use tables for the line cooling from molecules: H\(_2\)O, OH and CO from Neufeld and Kaufman (1993). H\(_2\) line cooling is treated thanks to the level by level time-dependent treatment of
all populations. Photo-electric heating from dust grains and cosmic ray ionization heating are also included.

### 4.1.3 Transverse stationary shock wave

The stationary hypothesis is a simplified way to analyze the shock structure. An MHD shock wave is called stationary if its structure does not change in time, so that the time derivative in all conservation equations above vanishes in the frame of motion of the structure. In addition, the MHD shock wave is called transverse if the direction of the ambient magnetic field is perpendicular to the direction of the shock propagation.

#### 4.1.3.1 Rankine-Hugoniot relation

For a single fluid, mass and momentum are conserved. The source terms $S$, $B$ and $A$, therefore, on the right hand side of Equation 4.3 and Equation 4.5 are equal to zero. In general, number density and energy can vary because of the neutral-neutral reactions, such as the collisional dissociation of $H_2$. However, those chemical collisional processes are all inelastic, for which the time (and distance) scales are larger compared to the corresponding elastic collision process. Therefore, the first few mean free-paths of the shock, where the viscous transition takes place, qualify as adiabatic, which means that the shock does not exchange energy with the shock’s ambient medium.

Owing to all of those approaches, we enable relations to be obtained between the pre-shock (upstream) and the post-shock (downstream) gas. Those relations are referred to as the Rankine-Hugoniot relations

\[
\begin{align*}
\rho_1 v_1 &= \rho_2 v_2 \\
\rho_1 v_1^2 + n_1 k_B T_1 + \frac{B_1^2}{8\pi} &= \rho_2 v_2^2 + n_2 k_B T_2 + \frac{B_2^2}{8\pi} \\
\left(\frac{1}{2}\rho_1 v_1^2 + \frac{\gamma}{\gamma-1} n_1 k_B T_1 + \frac{B_1^2}{4\pi}\right) v_1 &= \left(\frac{1}{2}\rho_2 v_2^2 + \frac{\gamma}{\gamma-1} n_2 k_B T_2 + \frac{B_2^2}{4\pi}\right) v_2 \\
B_1 v_1 &= B_2 v_2
\end{align*}
\]

where the subscripts (1) and (2) represent the pre-shock and the post-shock gas, respectively; and $\gamma$ adopts the value 5/3. The combination of equations 4.30-4.33 yields an
equation for the compression ratio $\rho_2/\rho_1$ across the adiabatic shock front

$$2(2-\gamma)b\left(\frac{\rho_2}{\rho_1}\right)^2 + \left[(\gamma - 1)M^2 + 2\gamma(1 + b)\right] \frac{\rho_2}{\rho_1} - (\gamma + 1)M^2 = 0. \quad (4.34)$$

In Equation 4.34, $M = v_s/c_1$ is the Mach number, which is the ratio of the shock speed to the isothermal sound speed in the pre-shock medium corresponding to the pressure $p_1 = n_1 k_B T_1$; and $b = B_1^2/(8\pi p_1)$ is the ratio of the magnetic pressure to the pre-shock pressure. The positive solution of the quadratic Equation 4.34 yields an analytical expression for the compression ratio of the gas caused by a discontinuity adiabatic shock:

$$\frac{\rho_2}{\rho_1} = \frac{2M^2(\gamma + 1)}{D + \sqrt{D^2 + 8bM^2(2-\gamma)(\gamma + 1)}} \quad (4.35)$$

where $D$ is

$$D = (\gamma - 1)M^2 + 2\gamma(1 + b). \quad (4.36)$$

When there is no magnetic field ($b_1 = 0$), the Mach number is

$$M^2 = \frac{\gamma + 1}{2} \frac{p_2}{p_1} + \frac{\gamma - 1}{2} \quad (4.37)$$

and Equation 4.34 gives the simplified expression of the compression ratio:

$$\frac{\rho_2}{\rho_1} = \frac{M^2(\gamma + 1)}{(\gamma - 1)M^2 + 2\gamma} = \frac{p_1 + hp_2}{p_2 + hp_1} \quad (4.38)$$

where $h = (\gamma + 1)/(\gamma - 1)$. When the value of $\gamma$ is 5/3, the value of $h$ is 4. In the shock region, the shock transition process leads to an increase of entropy, this increase consequently forces $p_2 > p_1$. We can demonstrate that the gas density in the post-shock region is always greater than in the pre-shock region from Equation 4.38.

Equation 4.38 also shows that in the extreme case where $M \gg 1$ (strong shock), $\rho_2/\rho_1 = h = 4$. Then, from Equation 4.30, we come up with

$$\frac{v_2}{v_1} = \frac{\rho_1}{\rho_2} = \frac{1}{4} \quad (4.39)$$

and the temperature change across the adiabatic front is given by

$$\frac{T_2}{T_1} = \frac{p_2 \rho_1}{p_1 \rho_2} = \left[\frac{p_2 + hp_1}{p_1 + hp_2}\right] \frac{p_2}{p_1}. \quad (4.40)$$
In the extreme limit case where \( p_2 \gg p_1 \):

\[
\frac{T_2}{T_1} = \frac{p_2}{k p_1} \rightarrow \infty
\]

\[
T_2 = \frac{5}{4 n_2 k_B} v_1^2
\]

(4.41)

To summarize, across the viscous discontinuity, the gas is compressed, the gas pressure and temperature increase, while the velocity of the gas decreases in the shock frame.

### 4.1.3.2 C-type and J-type shocks

As seen in Equation 4.30-4.33, the existence of the magnetic field affects the structure of the fluid. Two main approximations accordingly apply: single or multi-fluids.

**Single fluid flow: J-type shock wave**

If the magnetic field is weak or absent, all components (neutral, ion and electron) are assumed to have the same velocity and the fluid behaves like a single flow. The shock caused by the supersonic propagation is sometimes called “hydrodynamic” with an extra contribution from the magnetic pressure. If the speed of the shock is greater than the signal speed in the pre-shock medium. The latter cannot ”feel” the shock wave before it arrives. Across the shock front, the variables (pressure, density, velocity, etc.) of the fluid vary as a viscous discontinuity jump (the so-called J-type shock). After being heated, accelerated and compressed by the shock wave, the gas cools down through radiative emission.

**Multi-fluid flow: C-type shock wave**

If the magnetic field is significant, its interaction with the charged component (including the grains) leads to the multifluid situation, where the neutral and charged components have different velocities. The magnitude difference strongly depends on the collisional coupling efficiency between the neutral and charged fluids.

When the ionization fraction is small, the magnetosonic speed \( v_m \) in the charges in the direction of shock propagation is defined as

\[
v_m = \sqrt{c_s^2 + \frac{B^2}{4 \pi \rho_c}} \approx \frac{B}{\sqrt{4 \pi \rho_c}}
\]

(4.42)
where \( c_s \) and \( B^2 / 4\pi \rho_c \), the speed of sound and the Alfvén speed of the charged fluid, can be greater than the shock entrance velocity. Then a magnetic precursor forms upstream of the discontinuity, where the charged and neutral fluids dynamically decouple. The resulting friction between the two fluids heats up and accelerates the neutral fluid. If the intensity of the magnetic field keeps increasing, the precursor size also increases, and the neutrals are compressed sooner before the arrival of the shock front. This leads eventually to the disappearance of the discontinuity, and the shock variables change continuously (the so-called C-type shock). Because of friction between the neutral and charged components, the kinetic energy dissipation is a much more gradual process and is spread over a much larger volume.

Figure 4.1 illustrates the difference of the thermal profile between J-type and C-type shocks.
Chapter 1. 1D-Shock model: Paris-Durham shock code

4.1.4 Transverse non-stationary shock wave: CJ-type

In the previous section, the shock properties were described in the case of steady state \( \frac{\partial}{\partial t} = 0 \). This assumption is also satisfied if the time to reach the steady state is short compared to the age of the shock wave. Chièze et al. (1998) provided the time scale for a MHD shock reach steady state related to the shock speed, the initial gas density and the initial magnetic induction as

\[
\left| \frac{dv_n}{dz} \right|^{-1} \approx (n_i < \sigma v >_{in})^{-1}
\] (4.43)

However, the authors demonstrated that the shock speed and the magnetic induction have tiny influence on this time scale, of which is mostly influenced by the initial gas density. For instance, the time required to attend at steady state of a shock with the initial conditions of \( n_H = 10^3 \text{ cm}^{-3} \), \( v_n = 10 \text{ km s}^{-1} \) and \( B = 10 \mu \text{G} \) is about \( 5 \times 10^5 \text{ yr} \). That definitely raises a need to develop a non-stationary shock model. In addition, some previous studies pointed out the need of non stationary shock models to explain observational H\(_2\) emissions originating from outflows (i.e., Giannini et al. 2004; Gusdorf 2008; Gusdorf et al. 2015).

Smith and Mac Low (1997) studied the formation and time-evolution of a 1D C-type shock. In this simple case, the chemistry was ignored and the ionization fraction was a power law of gas density. They found that the evolution of C-shock approached the analytic steady-state solution in all cases. Chièze et al. (1998) also studied the time-dependent evolution of C-type and J-type shock, including the state of ionization of the gas by taking into account a chemical network. They showed that young C-type shocks looked like truncated steady-state: this yielded techniques to produce time-dependent snapshots from pieces of steady-state models (Flower and Pineau des Forêts, 1999, Lesaffre et al., 2004b). Following the approach of Lesaffre et al. (2004b) in the large compression case, the J-type front in a young C-type shock is thus inserted when the flow time in the charged fluid is equal to the age of the shock (so-called CJ-type shock). This approach is illustrated by Figure 4.2. The J-type shock is truncated when the total neutral flow time across the J-type part reaches the age of the shock (the same holds for young J-type shocks). As the shock gets older, the magnetic precursor grows larger and the velocity entrance into the J-type front decreases due to the ion-neutral drag. As a result, the maximum temperature at the beginning of the J-type front decreases with age, as illustrated in the bottom panel of Figure 4.2. If the magnetic field is strong enough, the J-type tail eventually disappears and the shock becomes stationary. The resulting structure forms a continuous transition between the pre-shock and the post-shock gas (a stationary C-type shock).
Figure 4.2: Velocity and thermal profiles of the non-stationary (CJ-type) shock. (Top) Velocity profile of a non-stationary shock with a shock speed of 15 km s$^{-1}$, a pre-shock density of $10^2$ cm$^{-3}$, and a dynamical shock age of 10$^4$ yr. (Bottom) Thermal profiles of the non-stationary shock (same shock speed and pre-shock density) for the various dynamical shock ages.
4.1.5 Influence of chemistry

Shocks play an important role in the interstellar gas evolution from both a dynamical and a chemical point of view. Through chemical processes, species are either formed or destroyed, ions and neutrals in fluid react, which affects the gas thermal balance. Pineau des Forêts et al. (1997) investigated the effect of the chemistry on the time-dependent shock calculations: when the chemistry is switched off, the ionization fraction changes only through the differential compression of the ionized and neutral fluids. So this fraction is the same in the pre-shock and post-shock regions. When the chemistry is accounted for, the ionization fraction is much lower which leads to a weaker ion-neutral coupling. Consequently, the shock region is broader than in the case of no chemistry as shown in the top panel of Figure 4.3. Therefore, the maximum of the temperature is also lower because the energy is dissipated over a larger region, as shown in the bottom panel of Figure 4.3. It is also clear that the dynamics and the chemistry are closely linked and that they need to be treated in parallel.

4.2 Input parameters

In this section, we present the input parameters of the Paris-Durham shock code, with typical ranges, as well as the initial species abundances and chemical networks.

4.2.1 Physical inputs

1- Type of shocks

- C represents the stationary C-type,
- J represents the stationary J-type,
- S represents the isochore evolution towards thermal and chemical steady state (for pre-shock computation).
- T represents the evolution at constant temperature and density.

2- Number of fluids

- 1 used for J and S single-fluid computations,
- 2 used for C computation, with neutral and charged fluid separated,
- 3 same as 2 but the temperature of the positive and negative fluids are decoupled (although they keep the same velocity).
Figure 4.3: Effect of chemistry. (Top) Ionization fraction predicted by a model in which \( v_s = 10 \text{ km s}^{-1}, n_H = 10^5 \text{ cm}^{-3} \) and \( B_0 = 25 \mu \text{G}. \) (Bottom) Corresponding temperature profile of the ionized and the neutral fluids (Pineau des Forêts et al., 1997).
3- Magnetic field
   - $b = B_0 (\mu G)/\sqrt{n_H} \text{ (cm}^{-3}\text{)},$ with $B_0$ the ambient traverse magnetic field.

4- Initial density of hydrogen nuclei (cm$^{-3}$)
   - $n_H = n(H) + 2n(H_2) + n(H^+) + \ldots$

5- Shock speed (km s$^{-1}$)

6- Initial difference in velocity (cm s$^{-1}$) between the ionized and neutral fluid: $\Delta v = 10^{-3}$ cm s$^{-1}$

7- Kinetic temperature of the gas: $T_0$ taken from the steady state computation.

8- Grain surface temperature: $T_g = 15$ K

9- Method of molecular cooling calculation (except $H_2$): Neufeld and Kaufman (1993)
L VG tables or simple analytic formula (low density regime).

10- Environment
   - cosmic ray ionization rate: $3 \times 10^{-17}$ s$^{-1}$
   - local radiation field: multiplicative factor with respect to the Draine (1978) field $G_0 = 1$
   - visual extinction of the incident radiation field: $A_v = 0.1$

11- $H_2$ parameters
   - initial value of the ortho/para ratio of $H_2$: usually O/P=3
   - number of rovibrational levels of $H_2$: usually 150 levels
   - number of $H_2$ transitions to be output: 50 lines
   - method of determination for the internal energy distribution of $H_2$ when it forms on grains, usually assumed proportional to the Boltzmann distribution at 17249 K (4.48eV/3).
   - method of determination for the kinetic energy of $H_2$ newly formed on grains, usually a third of the formation energy.

12- Parameters of the numerical methods
   - maximum number of integration steps: $10^5$
   - inverse of the collision cross-section to characterize the viscosity: $3 \times 10^{14}$ cm$^{-2}$
   - tolerance on DVODE’s numerical integration: $\epsilon = 10^{-8}$
• dynamical age (years) of shock in CJ-type shock.
• maximum evolutionary age (years) of the shock: \(10^6\) years. Note that if this parameter is lower than the dynamical age of shock, no CJ-type shock is calculated.

### 4.2.2 Chemical inputs

We use 134 chemical species consisting of neutrals, positive ions, negative ions and grains (mantles and cores), the list of which is given in Appendix G. The initial elemental compositions of the most abundant species are listed in Table 4.1. The net formation and destruction rate of the chemical species per unit volume is carried out by a chemical network with 1180 chemical reactions, including: cosmic-ray ionization or dissociation, cosmic-ray-induced desorption from grains, \(\text{H}_2\) formation on grains, three-body reactions on grain surfaces, sputtering of grain mantles, erosion of grain cores, adsorption onto grain surfaces, collisional dissociation of \(\text{H}_2\), all other reactions, and reverse (endoergic). The form of the rate coefficient varies from one reaction to another, but all the rate coefficients are described by three parameters \(\alpha, \beta, \gamma\), which are parameterized in the chemical network through an Arrhenius form: 

\[
k = \gamma \left(\frac{T}{300}\right)^\alpha e^{-T/\beta}.
\]

Table 4.2 shows the first five reactions of the full chemical network.
| element | Xtot | gas  | PAH  | Mantle | Core    |
|---------|------|------|------|--------|---------|
| H       | 1.000E+00 | 1.000E+00 | 1.800E-05 | 2.300E-14 |
| He      | 9.999E-02  | 9.999E-02  |           |         |
| C       | 3.549E-04  | 1.380E-04  | 5.400E-05 | 6.999E-15 | 1.629E-04 |
| N       | 7.939E-05  | 7.939E-05  |           | 3.000E-15 |
| O       | 4.419E-04  | 3.020E-04  | 1.400E-14 | 1.399E-04 |
| Mg      | 3.700E-05  | 9.999E-16  |           | 3.700E-05 |
| Si      | 3.707E-05  | 3.370E-06  | 3.000E-15 | 3.370E-05 |
| S       | 1.860E-05  | 1.860E-05  |           | 2.000E-15 |
| Fe      | 3.231E-05  | 1.500E-08  | 9.999E-16 | 3.230E-05 |
| G       | 4.627E-11  | 4.627E-11  |           |         |

Table 4.1: Initial elemental compositions of the most abundant species in the ISM (Flower and Pineau des Forêts 2003).

| R1 | R2 | P1 | P2  | P3 | γ  | α  | β   |
|----|----|----|-----|----|----|----|-----|
| H  | H  | H2 |     |    | 8.14E-17 | 0.5 |
| H  | e− | H+ | e−  | e− | 9.20E-10 | 0.5 | 157890.0 |
| H2 | e− | H2+| e−  | e− | 1.40E-09 | 0.5 | 179160.0 |
| H  | H+ | H+ | H+  | e− | 1.30E-13 | 0.5 | 157890.0 |
| H  | H3+| H3+| H+  | e− | 1.30E-13 | 0.5 | 157890.0 |

Table 4.2: First five reactions of the full chemical network. The full chemical network is given in Appendix H.
Chapter 5

BOW SHOCK MODEL

As in Gustafsson et al. (2010), we assume that the 3D bow shock is made of independent planar shocks. We actually neglect the curvature effects and the friction between different 1D shock layers, the gradients of entrance conditions in the planar shock models, and the possible geometrical dilution in the post-shock: our approximation is valid as long as the curvature radius of the bow shock is large with respect to the emitting thickness of the working surface.

5.1 Geometry and coordinate system

Let’s consider an axisymmetric 3D bow shock around a supersonic star (or a jet) traveling at the speed of $-u_0$ relative to an ambient molecular cloud assumed to be at rest. In the frame of the star, the impinging velocity of ambient gas is uniform and equal to $u_0$. The apex of the bow shock is at position A and the star at position O (Figure 5.1). The axis of symmetry (z-axis) along the direction (AO). The observer is assumed to stand in the (Oxz) plane. The axisymmetric shape of the bow shock is completely determined by the function $z = f(x)$. The local position along the planar shock can be specified by the angle between the incoming flow and the tangent to the surface $\alpha = \arcsin(u_\perp/u_0)$ (see Smith and Brand, 1990a, figure 1), and by the angle $\varphi$ between the radius and the x-axis in the (xy) plane of projection.

The impinging velocity can be expressed as $u_0 = t u_\parallel + n u_\perp = u_0(t \cos \alpha + n \sin \alpha)$, where $n(-\cos \alpha \cos \varphi, -\cos \alpha \sin \varphi, \sin \alpha)$ is the unit normal vector pointing inside the bow and $t(\sin \alpha \cos \varphi, \sin \alpha \sin \varphi, \cos \alpha)$ is the unit tangent vector along the working surface and directed away from apex. The effective shock speed at the local point is $v_s = u_\perp = u_0 \sin \alpha$. Away from the axis of symmetry, the effective entrance velocity into the shock
Figure 5.1: Morphology of a magnetized bow shock in the frame of a star or a jet. The direction of the magnetic field is expressed by the angles $\psi$ and $\phi$. The observer lies at an angle $i$ to the z-axis in the Oxz plane.

decreases down to the sound speed $c_s$ in the ambient medium. Beyond this point, the shock working surface is a cone of opening angle $\alpha_0 = \arcsin(c_s/u_0)$, wider as the terminal velocity is closer to the sound speed. Here, we mainly focus on the “nose” of the bow shock where $u_\perp > c_s$, and we neglect the very weak emission from these sonic conical “wings”, assuming that they fall outside the observing beam.

The orientation of the line-of-sight of the observer in the $(x, z)$ plane is defined by the inclination angle $i$: $\hat{\mathbf{i}}(\sin i, 0, \cos i)$. The ambient uniform magnetic field is identified by the obliqueness $\psi$ and the rotation $\phi$: $\mathbf{B}/B_0 = (\cos \psi \cos \phi, \cos \psi \sin \phi, \sin \psi)$. $\psi$ and $\phi$ are fixed for each bow shock.

### 5.2 Distribution of effective 1D-shock velocity

This section aims at computing the fraction $P(u_\perp)\,du_\perp$ of planar shocks with an entrance shock speed $u_\perp$ within $du_\perp$ in a given bow shock shape. This will help us building a model for the full bow shock from a grid of planar shocks.

Considering the shock geometry as described in section 5.1, we aim at obtaining the formula for the unit area $ds$ corresponding to these shocks as a function of $du_\perp$. 
Chapter 5. Bow shock model

The norm of a segment $dl$ on the $(x, z)$ section of the bow shock surface is:

$$dl = \sqrt{dx^2 + dz^2} = \sqrt{1 + f'^2(x)}dx. \quad (5.1)$$

Now, take that segment and rotate it around the $z$-axis, over a circle of radius $x$. The area ($ds$) of the bow shock’s surface swept by this segment can be expressed as:

$$ds = 2\pi xdl = 2\pi x\sqrt{1 + f'^2(x)}dx. \quad (5.2)$$

Note that the angle $\alpha$ defined in Figure 5.1 is also the angle between the segment $dl$ and the differential length $dz$ along the $z$-axis. The tangent of the angle $\alpha$ can then be set as

$$\tan \alpha = \frac{dx}{dz} = \frac{1}{f'(x)}. \quad (5.3)$$

The relationship between $\alpha$ and $u_\perp$ will be realized according to whether we consider the shock in the ambient medium or in the stellar wind or jet. Then, $ds$ can be obtained as a function of $du_\perp$ by replacing that relation into Equation 5.2. However, we will only focus here on the bow shock in the ambient material. In that case, the norm of the effective velocity (i.e., the effective normal velocity $u_\perp$) is related to the norm of the incident velocity $u_0$ through the angle $\alpha$

$$u_\perp = u_0 \sin \alpha \rightarrow \alpha = \arcsin\left(\frac{u_\perp}{u_0}\right). \quad (5.4)$$

$x$ can now be expressed as a function of $u_\perp$ by substituting Equation 5.4 into Equation 5.3:

$$\tan[\arcsin\left(\frac{u_\perp}{u_0}\right)] = \frac{1}{f'(x)} \rightarrow x = f^{-1}\{\cot[\arcsin\left(\frac{u_\perp}{u_0}\right)]\} = g(u_\perp). \quad (5.5)$$

In Equation 5.2, the unit area $ds$ of the shock is a function of the coordinate $x$, while in Equation 5.5, the coordinate $x$ is a function of the effective shock velocity $u_\perp$. To sum up, we can obtain $ds$ as a function of $u_\perp$:

$$ds(u_\perp) = 2\pi g(u_\perp)\sqrt{1 + \cot^2[\arcsin\left(\frac{u_\perp}{u_0}\right)]}g'(u_\perp)du_\perp$$

$$= \pi \sqrt{1 + \cot^2[\arcsin\left(\frac{u_\perp}{u_0}\right)] \ d[g^2(u_\perp)]} \quad (5.6)$$
Finally, the distribution function of shock velocities is simply defined as

\[ P(u_\perp) = \frac{ds(u_\perp)}{\int_{c_s} ds}, \tag{5.7} \]

where the integral of \( P(u_\perp) \) is normalized to unity. Note that the lower limit of the integral is the sound speed in the ambient medium. This implicitly assumes that we only focus on the “nose” of the bow shock, where \( u_\perp < c_s \). One could include the conical “wings” by adding a Dirac distribution \( \delta(u_\perp = c_s) \). Conversely, one could also narrow down the integration domain if the beam intersects a smaller fraction of the bow. We implemented this mathematical formulation numerically to compute the distribution \( P \) from an arbitrary input function \( f \). The results we obtained agree with those obtained using the analytical expressions when the shape assumes a power-law dependence \( z \sim x^{\beta} \) (see Appendix B for detail).

In an elegant and concise article, Wilkin (1996) derived an analytical description of the shape of a bow shock around a stellar wind when it is dominated by the ram pressure of the gas. When dust grains control the dynamics of the gas, the main forces are the gravitation pull and the radiation pressure from the star, therefore the shape of the shock should be very close to the grains avoidance parabola derived in Artymowicz and Clampin (1997). In fact, the ISM mixes gases and dust grains, so the actual bow shock shape should lie in-between.

If dust dominates, the bow shock shape is the Artymowicz parabola expressed as \( z = \frac{1}{4R_0} x^2 - R_0 \) with \( R_c = 2R_0 \) the curvature radius at apex, \( R_0 \) being the star-apex distance. If gas dominates, the bow shock shape follows the Wilkin formula \( R = \frac{R_0}{\sin \beta} \sqrt{3} \sqrt{1 - \theta \cot \theta} \) with \( R_c = 5/4R_0 \) the curvature radius at the apex and \( \theta \) the polar angle from the axis of symmetry as seem by star.

Finally, in the case of the tip of a jet, Ostriker et al. (2001) showed that the shape of the bow shock was cubic \( z = x^3/R_0^2 - z_j \) with an infinite curvature radius at apex \( (R_0 \) and \( z_j \) are length-scale parameters). Figure 5.2 displays the distributions obtained for various bow shock shapes. Note that low-velocity shocks (\( u_\perp \leq 15 \text{ km s}^{-1} \)) always dominate the distribution: this stems from the fact that the corresponding surface increases further away from the axis of symmetry, where entrance velocities decrease. The distribution for the cubic shape has a spike due to its flatness (infinite curvature radius) near the apex. The Wilkin shape has a cubic tail but a parabolic nose. In Figure 5.3 we display the dimensionless surface \( S/\pi R_0^2 \) where \( S \) is the total surface of the bow shock out to \( u_\perp = c_s \), and \( R_0 \) an estimate of the radius of the nose of the bow. For elongated shapes such as the parabolic shape, the total surface can be much bigger than the nose cross-section \( \pi R_0^2 \). We will subsequently essentially consider an ambient shock with a parabolic shape (Artymowicz shape).
Figure 5.2: Statistical distributions of 1D planar shock along the bow shock obtained for various bow shock shapes. These distributions are dominated by low-velocity shocks.

Figure 5.3: Total surface of the bow shock for various bow shock shapes and terminal velocities, in units of $\pi R_0^2$, where $R_0$ is the length-scale parameter of the bow (on the order of the nose’s curvature radius).
Chapter 5. Bow shock model

5.3 Distribution of effective magnetic field

The magnetic field decouples the ions from the neutral fluid in the shock. However, as discussed by Smith (1992), the effective magnetic field is the component of the field parallel to the shock surface. The vector of the magnetic field can be expressed as $\mathbf{B} = \mathbf{t}B_\parallel + \mathbf{n}B_\perp$, where the perpendicular component is defined by $B_\perp = \mathbf{n} \cdot \mathbf{B}$. If the homogeneous preshock density is $n_H$, the strength scale factor of the ambient uniform magnetic field is defined as $b_0 = B_0(\mu\text{G}) / \sqrt{n_H[\text{cm}^{-3}]}$. The component of the field parallel to the working surface (scale factor $b_\parallel = B_\parallel(\mu\text{G}) / \sqrt{n_H[\text{cm}^{-3}]}$) is therefore given by

$$\left(\frac{b_\parallel}{b_0}\right)^2 = \cos^2\alpha \sin^2(\varphi - \phi) + \left[\cos\psi \sin\alpha + \sin\psi \cos\alpha \cos(\varphi - \phi)\right]^2 \quad (5.8)$$

where the angles $\alpha$ and $\varphi$ monitor the position in the bow shock (this expression is actually valid regardless of the bow shock shape). Figure 5.4 displays how this component ($b_\parallel$) changes along the shock surface in a few cases. For each given direction of the ambient magnetic field ($\phi$, $\psi$ fixed), $b_\parallel$ actually varies along two directions: along the bow shock shape ($\varphi$ fixed, $\alpha$ varied), visualized in the top panel, and along the annulus surface at one position on the bow shock surface ($\alpha$ fixed, $\varphi$ varied), visualized in the bottom panel.

5.4 Grid of 1D-shock models

We set all the parameters to values corresponding to typical conditions encountered in the molecular interstellar gas in our Galaxy (Table 5.1). We assume that the ambient gas is initially at chemical and thermal equilibrium and we compute the initial state as in Lesaffre et al. (2013) by evolving the gas at constant density during $10^{12}/n_H$ yr. Our initial elemental abundances in the gas, grain cores and ice mantles are the same as in Flower and Pineau des Forêts (2003) (Table 4.1). We also include PAHs with ratio $n(\text{PAH})/n_H = 10^{-6}$. The irradiation conditions are for a standard external irradiation field ($G_0 = 1$) but an additional buffer of $A_v = 0.1$, $N_0(\text{H}_2) = 10^{20}\text{ cm}^{-2}$ and $N_0(\text{CO}) = 0\text{ cm}^{-2}$ is set between the source and the shock so that the gas is mainly molecular (Lesaffre et al., 2013). In our calculations, the atomic hydrogen fractions $n(H)/n_H$ are $7.85 \times 10^{-2}$, $5.94 \times 10^{-4}$ and $5.89 \times 10^{-6}$ for pre-shock gas densities of $10^2$, $10^4$ and $10^6\text{ cm}^{-3}$, respectively. These initial conditions at steady state are then used as pre-shock conditions to compute the grid of planar shock models.

The shock velocities range from 3 to 40 km s$^{-1}$ as in Lesaffre et al. (2013), with a step of $\Delta u = 1\text{ km s}^{-1}$. However, we take into account the effect of the finite shock age by
Figure 5.4: Variation of the effective transverse magnetic field $b_\parallel$ along the bow shock surface for various directions of $b$ (top) and a fixed direction depending on the position on an annulus circle (bottom).
| Parameter                | Value                       | Note                                      |
|--------------------------|-----------------------------|-------------------------------------------|
| $n_H$                    | $10^2 \text{cm}^{-3}$, $10^4 \text{cm}^{-3}$ | Pre-shock density of H nuclei             |
| $A_\nu$                  | 0.1                         | Extinction shield                         |
| $N_0(H_2)$               | $10^{20} \text{cm}^{-2}$   | Buffer H$_2$ column density               |
| $N_0(CO)$                | $0 \text{ cm}^{-2}$        | Buffer CO column density                  |
| $G_0$                    | 1                           | External radiation field                  |
| $\zeta$                  | $3.10^{-17} \text{ s}^{-1}$ | Cosmic ray flux                           |
| OPR                      | 3                           | Pre-shock H$_2$ ortho/para ratio          |
| $u_\perp$                | 3, 4, 5, ..., 40 km s$^{-1}$ | Effective shock velocity                  |
| $b_\parallel v_{m1}/u_\perp$ | 0, ..., 1                   | Range of $b_\parallel$ parameter for J-type shocks |
| $b_\parallel v_{m1}/u_\perp$ | 1, ..., $v_{m1}/3 \text{km} \text{s}^{-1}$ | Range of $b_\parallel$ parameter for CJ-type shocks |
| age $\times n_H$/100 cm$^{-3}$ | $10^2$, $10^3$, $10^4$, $10^5 \text{yr}$ | Shock age                                 |

Table 5.1: Main input parameters of model.

considering snapshots at 4 different values of age: $10^2$, $10^3$, $10^4$, and $10^5$ years for a density of $n_H = 10^2 \text{ cm}^{-3}$, and a hundred times shorter for a density of $n_H = 10^4 \text{ cm}^{-3}$. Note that the typical time to reach the steady-state in a C-type shock with $G_0 = 1$ is about $t_s = 10^6 \text{yr}/(n_H/10^2 \text{cm}^{-3})$ (with little or no magnetic field dependence Lesaffre et al., 2004a).

The projected value of the magnetic field parallel to the shock $B_\parallel$ varies along the shock surface, so we need to sample the range of attainable values in our grid. The first constraint for a shock to exist is that its entrance velocity $u_\perp$ be greater than the Alfvén velocity $v_A = B_\parallel / \sqrt{4\pi \rho} \approx b_\parallel \cdot 1.85 \text{ km s}^{-1}$ where we defined the dimensionless value of the transverse magnetic field using the standard scaling $b_\parallel = B_\parallel / \mu G / (n_H/\text{cm}^{-3})^{1/2}$. The condition $u_\perp > v_A$ translates as $b_\parallel < u_\perp / 1.85 \text{ km s}^{-1}$, and we use as upper limit of our grid $b_\parallel < b_{\parallel \text{max}} = u_\perp / 3 \text{ km s}^{-1}$ (Figure 5.5).

Another important parameter is the magnetosonic speed in the charged fluid (Equation 4.42) defined as the fastest signal speed in a partially ionized medium. Due to the low ionization degree in the molecular ISM, it is almost proportional to the local magnetization parameter: $v_m \approx \sqrt{B_\parallel^2 / 4\pi \rho_c} = b_\parallel v_{m1}$ where $v_{m1}$ is the magnetosonic speed obtained when the magnetization parameter is equal to unity. In our calculations, we find $v_{m1} = 18.5 \text{ km s}^{-1}$ or $v_{m1} = 19.2 \text{ km s}^{-1}$ for respective densities of $n_H = 10^2 \text{ cm}^{-3}$ or $n_H = 10^4 \text{ cm}^{-3}$. The charged fluid mass is dominated by the dust grains: the gas-to-dust ratio turns out to be $\rho / \rho_d = 180$ for the cores and mantle composition used in our simulations.
5.5 \( \text{H}_2 \) excitation diagram

The average column-density of a given excited level of \( \text{H}_2 \) along the bow shock can be expressed as:

\[
N_{vJ}^{\text{tot}}(age, u_0, b_0, \psi) = \int_0^{2\pi} \frac{d\varphi}{2\pi} \int_{e_x}^{u_0} P_{u_0}(u_\perp) N_{vJ}(age, u_\perp, b_\parallel) du_\perp
\]

(5.9)

where \( P_{u_0(u_\perp)} \) is the distribution computed in section 2 and \( N_{vJ}^{\text{tot}} \) and \( N_{vJ} \) are the column-densities of \( \text{H}_2 \) in the excited level \((v, J)\) in the whole bow shock and in each planar shock, respectively.

5.5.1 \( \text{H}_2 \) excitation in C-type and J-type shocks

A \( \text{H}_2 \) rovibrational level \((v, J)\) can be populated after a collision with another species, mainly \( \text{H}_2 \), H, He and \( \text{e}^- \) provided that the temperature yields more energy per particle than the energy level \( E_{vJ} \). In a J-type shock, the sudden surge of viscous heat in the adiabatic shock front easily leads to high temperatures \((T_J = 53K(u/km\ s^{-1})^2, \text{Lesaffre et al. (2013)})\) which are able to excite high energy levels. The plots a and b of Figure 5.6
show the level populations for young ages, where even CJ-type shocks are dominated by their J-type tail contribution. These figures illustrate the threshold effect for two different energy levels: their population quickly rises and reaches a plateau when \( u > u_{vJ} \), with \( u_{vJ} \) a critical velocity depending on the energy level. Note the weak dependence of the plateau on the shock magnetization for J-type shocks, as magnetic pressure only marginally affects their thermal properties. The critical velocity \( u_{vJ} \) mainly depends on the energy level \( (E_{vJ} \simeq k_B T_{J}) \) and only weakly depends on the magnetization.

On the other hand, C-type shocks dissipate their energy through ion-neutral friction, a process much slower than viscous dissipation: at identical velocity, C-type shocks are much cooler than J-type shocks, but their thickness is much larger. C-type shocks dominate the emission of old CJ-type shocks, when the J-type front contribution almost disappears (Figure 5.6c in C-type shocks). Due to their low temperature, high energy levels can never be populated (Figure 5.6d). This enhances the threshold effect, with a discontinuous jump at \( u = b v_{m1} \). On the contrary, energy levels lower than \( k_B T_C \), with \( T_C \) the typical temperature of a C-type shock, will be much more populated in a C-type shock than in a J-type shock due to the overall larger column-density. This is illustrated in the Figure 5.6c for a low energy level. The discontinuous jump at \( u = b v_{m1} \) becomes a drop instead of a surge and a peak appears in the level population. Magnetization in C-type shocks controls the compressive heating which, in turn, impacts the temperature: excitation of H\(_2\) low-energy levels in C-type shocks decreases systematically with larger magnetization, but the effect remains weak within C-type shocks. However, the magnetization is important insofar as it controls the transition between C-type and J-type shocks, which have very different emission properties.

To summarize, at a density of \( n_H = 10^2 \text{ cm}^{-3} \), the column density excitation of a given H\(_2\) level follows a threshold in velocity after which a plateau is reached, with little or no magnetic field dependence. However, low energy levels at old ages, for velocities below the magnetosonic speed, can be dominated by C-type shock emission. In that case, the H\(_2\) level population peaks at the magnetosonic speed before reaching a plateau. Therefore, H\(_2\) emission in bow shocks is likely to be mostly dominated by J-type shocks.

At higher density of \( 10^4 \text{ cm}^{-3} \), the picture is essentially unchanged, except for the effect of H\(_2\) dissociation which is felt when the velocity is larger than the H\(_2\) dissociation velocity \( (v_s \sim 25 \text{ km s}^{-1}) \): the value of the plateau decreases beyond this velocity (see the right half of each panel in Figure 5.7, which is in other respects similar to Figure 5.6). At even higher densities, H\(_2\) dissociation completely shuts off H\(_2\) emission in J-type shocks, and we reach a situation where the bow shock emission is dominated by C-type shocks, as in Gustafsson et al. (2010).

As demonstrated, \( N_{vJ} \) sharply increases as a function of \( u_\perp \) at a given threshold velocity \( u_{vJ} \) before reaching a plateau. We also showed that the statistical distribution of shock
Figure 5.6: Overview of our model results for a pre-shock density $n_H = 10^2$/cm$^3$. The natural logarithm of the integrated column-densities of H$_2$ populations is normalized by their statistical weight. They are given as a function of the velocity $u$ for various values of the magnetic field parameter $b_\parallel$. Left panels are for the level $(v, J) = (0, 3)$, the upper level of the 0-0S(1) line and the right panels are for the level $(v, J) = (1, 3)$, the upper level of the 1-0S(1) line. Upper panels are for a young age of $10^3$ yr while bottom panels are nearly steady-state at an age of $10^5$ yr. In each panel, the symbol ‘o’ marks the transition between CJ-type shocks (on the left-hand side) and J-type shocks (on the right hand side), when the velocity $u$ is equal to the magnetosonic speed $b u_{m1}$.

speeds $P(u_\perp)$ in a bow shock was steeply decreasing as a function of $u_\perp$. As a result, the product of the two peaks at around $u_{vJ}$ and its integral over $u_\perp$ is a step function around $u_{vJ}$ (Figure 5.8). This situation is reminiscent of the Gamow peak for nuclear reactions. Then, $N_{vJ}^{\text{tot}}(u_0)$ tends to a finite value when $u_0$ is much greater than the threshold velocity $u_{vJ}$. The final value depends both on magnetization and age.
5.5.2 Effect of the terminal velocity

Figure 5.9a shows the influence of the terminal velocity on the excitation diagrams of H₂ at an age of 10⁴ yr. As expected, the excitation diagram saturates at large velocity, when \( u_0 \) is larger than all the individual \( u_{v,J} \) of the levels considered. That saturation occurs quicker at low energy levels, as the corresponding critical velocity is lower.

5.5.3 Effect of the ambient density

Figure 5.9b illustrates the effect of density on the excitation diagram. Roughly speaking, the column-densities are proportional to the density, but in this example (40 km s⁻¹ bow shock), higher energy levels are subject to H₂ collisional dissociation, and they are slightly less populated relative to their low energy counter part.
Figure 5.8: Illustration of the “Gamow-peak” effect on the integration of the total column densities of the H\textsubscript{2} level $\langle v, J \rangle = (1, 3)$ in a bow shock with terminal velocity $u_0 = 30$ km s\textsuperscript{-1}, $n_H = 10^2$ cm\textsuperscript{-3}, and the age is $10^5$ yr.

5.5.4 Effect of shock age

At young ages, shocks are dominated by the emission properties of J-shock: as time passes, C-type shocks increase the emission of low energy levels and the excitation diagram of the bow shock is slightly steeper at the origin (Figure 5.9c). Interestingly, the energy level just above 2000K does not seem to be affected by age (it is also weakly affected by all of the other parameters) and all the curves converge on this point.

5.5.5 Effect of shock shape

As mentioned in section 5.2, the shape of bow shocks affects the velocity distribution and the relative weight of the large velocities increases when one moves from a parabola to a Wilkin shape. As a result, a bow shock with a Wilkin shape has more excited high energy levels than a parabolic bow shock (Figure 5.9d).
Figure 5.9: Excitation diagrams of H$_2$ showing the effect of varying some of the parameters of the model. The reference model ($n_H=10^2$ cm$^{-3}$, age=10$^5$ yr, $b_0=1$, $\Psi=0$, parabola shape, $u_0=40$ km s$^{-1}$) is displayed in blue. The circle symbols correspond to $v = 0$ (pure rotational levels) and the square symbols to $v = 1$. 
5.5.6 Effect of ambient magnetic field

The magnetic field tends to shift the transition between C-type and J-type shocks in the bow shock to larger velocities. At early age, it does not matter much, since both C-type and J-type shocks are dominated by J-type shock emission. At later ages, though, the low energy levels get an increasing contribution from C-type shocks and see their excitation increase. Conversely, high energy levels are less excited because the overall temperature of the shock decreases (Figure 5.9e). The orientation of the magnetic field azimuthally affects the range of values of $b$ (as $\varphi$ varies) but its main systematic effect is to shift the maximum magnetization from low velocities to large velocities as it gets more and more perpendicular to the axis of symmetry (Figure 5.4). Figure 5.9f shows the differential effect caused by varying the angle $\Psi$: tending $\Psi$ to $0^\circ$ amounts to increasing $b$ (high energy levels are less excited, whereas low energy levels are more excited). The resulting change is subtle but we show below that it might still be probed by observations.

5.5.7 Bias between 1D- and 3D-shock models

Observations often consider low energy transitions (pure rotational or low vib-rotational levels): although we included the first 150 levels in our calculations, here we mainly consider the levels with an energy up to $10^4$K. The two lowest rotational states (J=0 and 1) are, of course, unobservable in emission. The *James Webb Space Telescope* (JWST) will observe pure rotational transitions up to energies of about 5900K (seven levels involved). This is similar to the performances of the *Infrared Space Observatory* (ISO) and the *Spitzer* telescope. These two telescopes that have been used to observe shocked regions generate excitation diagrams and maps around Young Stellar Objects (YSOs) (i.e., Giannini et al. 2004; Neufeld et al. 2009) or supernova remnants (SNRs) (i.e., Cesarsky et al. 1999; Neufeld et al. 2014) shocks. The AKARI mission has also been used for similar purposes in SNRs environments (i.e., Shinn et al. 2011). The JWST will also target rovibrational transitions. Finally, the *Echelon-Cross-Echelle Spectrograph* (EXES) on board the *Stratospheric Observatory For Infrared Astronomy* (SOFIA) operating between 4.5 and 28.3 $\mu$m (DeWitt et al., 2014) should allow observations of pure rotational transitions of H$_2$, but no program has been explicitly dedicated to the observation of shocked H$_2$ with this instrument so far.

Most observations are unable to resolve all details of a bow shock, and the beam of the telescope often encompasses large portions of it, therefore mixing together planar shocks with a large range of parameters. However, it is customary to use 1D models to interpret observed excitation diagrams. In addition, previous work (NY08; Neufeld et al. 2009;
Neufeld et al. 2014) have also shown that statistical equilibrium for a power-law temperature distribution $T^{-b_{SE}} \, dT$ could be quite efficient at reproducing the observed $\text{H}_2$ pure rotational lines (see section 2.5). We thus seek to explore how accurately these two simple models perform compared to 3D bow shocks. We consider the worst case scenario where the whole nose of a parabolic bow shock is seen by the telescope: the effective entrance velocity $u_\perp$ varies from the speed of sound $c_s$ (in the wings of the bow shock) to the terminal velocity $u_0$ (at the apex of the bow shock).

The following $\chi$ function is used to estimate the distance between 1D and 3D models:

$$\chi^2 = \frac{1}{L} \sum_{v,j} \left[ \ln \left( \frac{N_{vj}^\text{tot}}{g_{vj}} \right) - \ln \left( \frac{N_{vj}^u}{g_{vj}} \right) - C \right]^2$$

with $L$ the number of observed rovibrational levels $(v,j)$, and $g_{vj}$ the statistical weight of each level $(v,j)$. The constant $C$ reflects the fact that the beam surface at the distance of the object may not match the actual emitting surface of the bow-shock, either because of a beam filling factor effect or because the bow-shock surface is curved. We assume here that the observer has a perfect knowledge of the geometry and we take $C = 0$, which means that the 1D shock model has the same surface as the 3D bow-shock to which it is compared with. The best 1D model and power-law assumption selected is the one yielding the smallest $\chi^2$ value on our grid of 1D models.

Figure 5.10 shows the result of the fit on a 30 km $s^{-1}$ bow shock at age $10^5$ years, density $n_{H} = 10^2 \, \text{cm}^{-3}$, and magnetization parameter $b_0 = 1$ ($\Psi = 90^\circ$). 1D models have the same parameters (same age, pre-shock density and $b_\parallel = 1$) except the entrance velocity $u_\perp$. We find that the best velocity is either 7 or 13 km $s^{-1}$ depending on the range of lines considered. This is way below the terminal velocity and this illustrates again the fact that the resulting 3D excitation diagram is dominated by low velocity shocks. As a consequence, the use of higher energy lines reduces the bias, and a cubic shape for the bow shock yields less bias towards low velocity than a parabolic shape (not shown here). In the left hand sides of the panels (b)-(d), the resulting $\chi^2$ is around one in all cases: it corresponds to an average mismatch of about a factor of 3 between the 3D and 1D column-densities, a common result when comparing 1D models and observations.

Figure 5.11 systematically explores this bias as a function of the bow shock terminal velocity: the best 1D model usually has an entrance velocity smaller than the terminal velocity of the 3D bow-shock. Moreover, when the 3D excitation diagram saturates at large $u_0$, the best 1D model does not change.

Following the approach of NY08 (described in section 2.5), we calculate the $\text{H}_2$ levels population in statistical equilibrium for temperatures ranging from 100K to 4000K and we convolve this with a power-law distribution of the gas temperature. We explore
Figure 5.10: Results of the fit of 1D models and statistical equilibrium approximations to a 3D bow shock. (a-b) Transitions with upper level $E_{v,j} < 5900$ K (JWST-like) are used. (c-d) Fitted transitions have $5900 < E_{v,j} < 10000$ K. (a-c) Comparison of the excitation diagrams of the bow shock to the best 1D fit and the best NY08 fit, (b-d) standard deviation of the natural logarithm difference between the two diagrams ($\chi = \sqrt{\chi^2}$) as the entrance velocity in the 1D model and the power-index in NY08 assumption vary. The bow shock parameters are: pre-shock density $10^2$ cm$^{-3}$, $b_0 = 1$, $\Psi = 90^\circ$, and the age is $10^5$ yr. Connected circle symbols all have $v = 0$ (pure rotational levels) while square symbols have $v = 1$.

power-indices ($b_{SE}$) varying from 3 to 6 (as in NY08) with steps of 0.2. We confirm that that the NY08 approximation performs very well in the low energy regime of pure rotation. In the case displayed in Figure 5.10(a), the optimal power-index is 3.6, close to the estimation of 3.77 for parabolic bow-shocks calculated by equation (4) in NY08. However, Figure 5.10(c) shows that this simple approach fails for higher energy vibrational or rotational levels.

We then turn on recovering magnetization from 1D models. We first fix the terminal velocity of the bow shock to $u_0 = 40$ km s$^{-1}$ and explore several values of the magnetization $b_0$, while keeping $\Psi = 90^\circ$. Once the best matching 1D velocity is found, we further let the magnetization parameter $b$ of the 1D model vary freely and explore which value best fits the 3D model (while keeping $u_\perp$ fixed). The result of this second adjustment is shown in Figure 5.12: the magnetization parameter of the best 1D model is only slightly below
\[ n_H = 10^2 \text{ cm}^{-3}, b_\parallel = 1 \]

and represents a good match to the original magnetization parameter of the bow shock. Next, we assume that a priori information about the bow shock velocity (usually by looking at some molecular line width, for example) is available. We now fix \( b_0 = 1 \) for the underlying 3D model and assume that \( u_\perp = u_0 \) in the 1D models while searching for the best \( b_\parallel \) value. The retrieved magnetization parameter is usually too high, which may lead to an overestimation of the magnetization parameter when the dynamics have been constrained independently.

### 5.6 H\(_2\) line shape

Smith and Brand (1990c) pioneered the study of the emission-line profile of molecular hydrogen from a simple C-type bow shock. We revisit their work with our models that better takes into account shock age, charge/neutrals momentum exchange, cooling/heating functions, the coupling of chemistry to dynamics, and the time-dependent treatment of the excitation of H\(_2\) molecules. We also introduce line broadening due to the thermal Doppler effect.
Figure 5.12: Magnetization bias between 1D and 3D models. The top panel is at $u_0 = 40 \text{ km s}^{-1}$ and for each value of $b_0$, it gives the best $b_\parallel$ after the best $u_\perp$ has been determined. The bottom panel is at $b_0 = 1$ and for each value of $u_0$, it gives the best matching $b_\parallel$ when $u_\perp = u_0$ is assumed. Symbols are the same as in Figure 5.11. The remaining parameters of the bow shock are the same as in Figure 5.10.
In the shock’s frame, the velocity of the gas equals 
\[ v(r, u_\perp, \varphi) = \hat{t} u_\parallel + \hat{n} u(r, u_\perp, b_\parallel), \]
where \( r \) is the distance within the shock thickness (orthogonal to the bow shock surface) and \( u(r, u_\perp, b_\parallel) \) is the shock orthogonal velocity profile as computed in the 1D model. Because of the large compression, the shock frame is moving very slowly with respect to the star, which we adopt as the observer’s frame. In the observer’s frame, the emission velocity becomes
\[
\begin{align*}
v_{\text{obs}} &\sim v = v - u_0 + u_0 \\
&= \hat{n} u(r, u_\perp, b_\parallel) - \hat{n} u_\perp + u_0 \\
&= \hat{n} u_\perp (\xi - 1) + u_0
\end{align*}
\]
where \( 0 \leq \xi(r, u_\perp, b_\parallel) \leq 1 \) is the ratio between the local velocity \( u(r, u_\perp, b_\parallel) \) to the orthogonal entrance velocity \( u_\perp \).

However, the observer only senses the component along the line of sight: \( v_{\text{obs}} \hat{l} \) with \( \hat{l} \) a unit vector on the line of sight, pointing towards the observer. Adopting the geometric symmetry, that unit vector relates to the viewing angle \( i \) as
\[
\hat{l} = \sin(i) \hat{i} + \cos(i) \hat{k}
\]
where \( \hat{i}, \hat{k} \) are the unit vectors on the x and z axes.

When this is expressed in the observer’s frame, the emission velocity becomes
\[
\begin{align*}
u_{\text{rad}} &= -v_{\text{obs}} \hat{l} \\
&= \hat{n} u_\perp (1 - \xi) \hat{l} - u_0 \hat{l} \\
&= 0.5 \ u_0 (\xi - 1) \cos(\varphi) \ \sin(2\alpha) \ \sin(i) + \ (1 - \xi) \frac{u_\perp}{u_0} \cos(i) - u_0 \cos(i)
\end{align*}
\]
with \( \alpha \) defined at Equation 5.4, \( u_\perp / u_0 = \sin \alpha \) and we have used \( \hat{n} \) at above section 5.1.

We assume the \( \text{H}_2 \) emission to be optically thin. Then the line profile is defined by integration over the whole volume of the bow shock, including the emission coming from each unit volume inside each planar shock composing the bow shock. The line emission at velocity \( V_r \) can be computed as follows:
\[
\begin{align*}
f(V_r, i) &= \int_{u_\perp} P(u_\perp) du_\perp \int_\varphi \frac{d\varphi}{2\pi} \\
&\quad \int_r d\rho \frac{R_0^2}{\sqrt{2\pi\sigma_T(r, u_\perp, b_\parallel)}} \epsilon(r, u_\perp, b_\parallel) e^{-\frac{[v_{\text{rad}}(r, u_\perp, b_\parallel)-V_r]^2}{2\sigma_T^2(r, u_\perp, b_\parallel)}}
\end{align*}
\]

\( \sigma_T \) is the temperature and \( \epsilon \) is the emission coefficient.
which includes Doppler broadening with $\sigma_T^2(r, \alpha) = \left(\frac{k_B}{m_{H_2}}\right) T_{H_2}(r, u_\perp, b_\parallel)$, the thermal velocity of the $H_2$ molecule. Note that the azimuthal angle $\varphi$ occurs both in the expression of $b_\parallel$ (see Equation 5.8) and in the projection of $v_{\text{obs}}$ onto the line-of-sight direction $\hat{l}$.

### 5.6.1 Effect of viewing angle

Figure 5.13a shows the effect of the viewing angle $i$ on the 1-0S(1) line shape. When the observer looks at the bow-shock from the point of view of the star ($i = 0^\circ$), all the emission is blue-shifted, with a stronger emission at a slightly positive velocity, coming from the part of the shock structure closest to the star, close to the J-type front where this line is excited. As $i$ increases, the line of sight intercepts two sides of the working surface, one going away and the other going towards the observer. The line profile then becomes doubly peaked. We checked that the integrated line emission did not vary with the viewing angle.

### 5.6.2 Effect of shock age

Figure 5.14a shows how the age affects the 1-0S(1) line profile at the viewing angle $i=60^\circ$. As the shock becomes older, the J-tail entrance velocity decreases: this explains why the two peaks of the line profile get closer to each other as age proceeds. The velocity interval between the two peaks is proportional to the entrance velocity in the J-type tail of the shocks. Furthermore, as the entrance velocity decreases, the temperature inside the J-shock decreases accordingly and the Doppler broadening follows: the line gets narrower as time progresses. The width of the 1-0S(1) could thus serve as an age indicator, provided that the shock velocity is well known.

The 0-0S(1) line corresponds to a much lower energy level than the 1-0S(1) line: while the 1-0S(1) is sensitive to temperature and shines mostly around the J-type front, the 0-0S(1) line emits in the bulk of the shock, where gas is cooler. Since the 0-0S(1) line probes a colder medium, the resulting profiles are much narrower (Figure 5.13b). For early ages (100 and 1000 yr), one can however still notice the double peak signature of the J-front (Figure 5.14b). Because at these early ages the temperature in the magnetic precursor is much colder than the transition’s upper level temperature of 1015 K for level (0,3), the 0-0S(1) line is shut off in the magnetic precursor (see the bottom panel of Figure 4.2, for example) and it therefore probes the J-shock part.
Figure 5.13: Line profiles of a whole bow shock parameterized by \( u_0 = 40 \text{ km s}^{-1} \), age = \( 10^2 \) years, \( b_0 = 1 \) and \( \phi = 0^\circ \). (a) for the H$_2$ 1-0S(1) line and (b) for the H$_2$ 0-0S(1) line.
Figure 5.14: Line profiles of a whole bow shock parameterized by $u_0 = 40 \text{ km s}^{-1}$, $i = 60^\circ$, $b_0 = 1$ and $\phi = 0^\circ$. (a) for the H$_2$ 1-0S(1) line and (b) for the H$_2$ 0-0S(1) line.
Chapter 6

BOW SHOCK MODELS TO INTERPRET OBSERVATIONS

6.1 $\text{H}_2$ excitation diagram

In this section, we briefly show how 3D bow shock models can be used to interpret and constrain the parameters of observations.

6.1.1 BHR71

Located at a distance of about 175 pc (Bourke et al., 1995), BHR71 is a double bipolar outflow (Bourke et al. 1997, Bourke 2001) emerging from a Bok Globule visible in the southern sky. The two outflows are spectrally distinguishable (Parise et al., 2006). Their driving protostars, IRS 1 and IRS 2, have luminosities of 13.5 and 0.5 $L_\odot$ (Chen et al., 2008) and are separated by about 3400 AU. For this double star system, the time since collapse has been evaluated to about 36000 yr (Yang et al., 2017). Many observations have been performed from infrared to sub-millimeter wavelength ranges. Bright HH objects HH320 and HH321 have been detected (Corporon and Reipurth, 1997), as well as chemical enhancement spots (Garay et al., 1998) and several other knots of shocked gas (Giannini et al., 2004). By combining $\text{H}_2$ observations performed by Spitzer (Neufeld et al. 2009, Giannini et al. 2011) and SiO observations obtained from the APEX telescope, Gusdorf et al. (2011) were able to characterize the non-stationary CJ-type shock waves propagating in the northern lobe of the biggest outflow. They more tightly constrained the input parameters of Paris-Durham shock models by means of successive observations of low- to higher-$J_{up}$ CO (Gusdorf et al. 2015) using APEX and SOFIA. The most recent
Table 6.1: Parameters that best reproduce the excitation diagram in BHR71. We also give a 3σ uncertainty range for the parameter Ψ (see text).

| Parameter | Value          | Description                                      |
|-----------|----------------|--------------------------------------------------|
| $n_H$     | $10^4$ cm$^{-3}$ | Pre-shock density of H nuclei                    |
| age       | $10^3$ yr      | Shock age                                       |
| $Δu_⊥$    | 21-23 km s$^{-1}$ | Range of $u_⊥$                                  |
| $b_0$     | 1.5            | Strength of the magnetic field                   |
| $ψ$       | $-50° \pm 20°$ | Orientation of the magnetic field                |
| $u_0$ and $β$ | N.A.  | Bow shock terminal velocity and shape are irrelevant because of the narrow range of velocities |

studies based on *Herschel* observation report the presence of an atomic jet arising from the driving IRS1 protostar (Nisini et al. 2015, Benedettini et al. 2017). This does not challenge the existence of a molecular bow-shock around the so-called SiO knot position in the northern lobe of the main outflow, where most attempts have been made to compare shock models with observations (Gusdorf et al. 2011, 2015, Benedettini et al. 2017). These studies have placed constraints on shock models of the H$_2$ emission over a beam of 24" centered on this position: pre-shock density $n_H = 10^4$ cm$^{-3}$, magnetic field parameter $b = 1.5$, shock velocity $v_s = 22$ km s$^{-1}$, and age of 3800 years. The influence of the external ISRF or from the driving protostar was neglected, with an equivalent $G_0$ factor set to 0. The excitation diagram that was used can be seen in Figure 6.1, where the large error-bars reflect the uncertainty on the filling factor and the proximity of the targeted region to the edge of the *Spitzer*-IRS H$_2$ map.

Here we attempt to reproduce the same H$_2$ emission data around the SiO knot position as in Gusdorf et al. (2015). To fit a 3D model to this data, we should in principle adjust all the parameters in Table 6.1, which would be a bit tedious and very likely underconstrained by the observations. Instead, we started up from already published parameters and expanded around these values. We hence use a narrow range of velocities around $u_0 = 22$ km s$^{-1}$, $b_0 = 1.5$ and $n_H = 10^4$cm$^{-3}$ as indicated by Gusdorf et al. (2015). These authors found an age of 3800 yr, so we took our grid models at an age of 1000 yr, as $10^4$yr would not be compatible with the extent of the shock. A speed of 22 km s$^{-1}$ during 1000 yr already results in a shock width of 0.02 pc, about the same size of the beam (24" at 200pc according to Gusdorf et al. (2015)), although the H$_2$ lines emission region is a factor of a few smaller.

Figure 6.1 illustrates the comparison between our models and the observational values. We first restrict the velocity range in the bow shock velocity distribution to the narrow interval [21,23] km s$^{-1}$ that is close to the solution of Gusdorf et al. (2015). This also
accounts for the fact that the beam selects a local portion of the bow-shock and one might expect to find a privileged velocity.

First, we examine the case $\psi = 90^{\circ}$ when the magnetization is close to $b_0$ and is uniform throughout a transverse annulus of the bow-shock. Technically this is still a 3D model, but it is very close to the model in our grid of planar shocks with similar parameters because we use a very narrow range of velocities combined with uniform magnetization. The excitation diagram for this model is noted as the blue triangles in Figure 6.1. Although it slightly differs from the best model of Gusdorf et al. (2015), it is not much further away from the observational constraints ($\chi = 1.0$ in the model in Gusdorf et al. (2015) and $\chi = 1.5$ in our model at $\psi = 90^{\circ}$).

Second, we leave the orientation of the magnetic field $\Psi$ free and we find the best model at $\psi = -45^{\circ}$: this greatly improves the comparison with observations ($\chi = 0.2$). In particular, the curvature of the excitation diagram that was difficult to model, is now almost perfectly reproduced. At this orientation, the model is a mixture of planar shocks with
transverse magnetization between \( b_0 \) and a small minimum value. Because we limited the velocity to such a narrow range, this model is effectively a 2D model.

Third, we checked that increasing the velocity range, changing the shock shape, or limiting the integration range for the angle \( \varphi \) (to account for the fact that the observational beam probably intersects only one flank of the bow shock) did not improve the fit: the interpretation capabilities of our 3D model seems to be reached. Table 6.1 sums up our constraints on the parameters of our model. We estimate 3-\( \sigma \) error bars for \( \Psi \) by investigating the shape of the \( \chi^2 \) well around the best value: we vary \( \Psi \) with all other parameters kept fixed and we quote the range of values where \( \chi^2 \) is below four times its minimum value.

Finally, we checked the NY08 approximation. As mentioned in subsection 5.5.7, that simple assumption surprisingly works well in the case of low pure rotational excitation. Figure 6.2 shows the best fit from the NY08 assumption with the value of the power-index at \( b_{SE} = 2.6 \), consistent with the value 2.5 in Neufeld et al. (2009) for the same object. The accuracy obtained as close to the data as our 3D model, with \( \chi = 0.2 \).
6.1.2 Orion BN-KL outflow

The BN-KL region in the Orion molecular cloud (OMC-1) is one of the well studied massive star forming regions. A central young stellar object generates a strong outflow that shocks the surrounding gas and yields a wealth of H$_2$ infrared emission lines previously observed by Rosenthal et al. (2000). These authors however indicated that the full range of H$_2$ level population could not be reproduced by a single shock model. In fact, Le Bourlot et al. (2002) showed that only a mixture between two C-type shock models could account for the population of both the low and the high energy levels (see section 2.3). In this work, we try to reproduce the observed excitation diagram of H$_2$ and strongest H$_2$ 1-0S(1) line profile from the OMC-1 Peak1 with one of our bow shock models.

We ran a new grid of models at the pre-shock conditions in Orion, $n_H = 10^6$ cm$^{-3}$ (White et al. 1986, Brand et al. 1988, Hollenbach and McKee 1989, Kaufman and Neufeld 1996, Kristensen et al. 2008). We limited the age to 1000 yr, which roughly corresponds to the dynamical age of the outflow (Kristensen et al., 2008). At these densities, the shocks should have reached steady-state long ago.

Then we explore the parameter space of all possible bow-shocks and seek the best fitting model. We considered $u_0$ between 20 and 100 km s$^{-1}$ and we varied $b_0$ from 1 to 6 with step 0.5. For each value of $b_0$, we let the angle $\psi$ vary from 0° to 90° with step 5°. Finally we explore the shape of the shock for $\beta$ in the interval from 1.0 to 3.0 with step of 0.2.

In the simplified case, we compute the $\chi^2$ for the 17 pure rotational transitions, with the vibrational levels $v = 0$ among the 55 transitions which have been measured, discarding the upper limits (table 3 of Rosenthal et al. 2000). The parameters that best fit the excitation diagram are listed in Table 6.2. We also provide an estimation of the 3$-\sigma$ uncertainty range for some parameters by investigating the shape of the $\chi^2$ well around the best value, as we did above for the parameter $\psi$ in the case of BHR71. The best model convincingly reproduces most of the lines ($\chi = 0.4$), as long as the terminal velocity is greater than 30 km s$^{-1}$. The comparison to the observations is displayed in Figure 6.3: both the low and high energy regimes of the excitation diagram are simulated by the same model. Two best matching models found by Rosenthal et al. (2000), which are a mixture of two C-type shock models from Kaufman and Neufeld (1996) and a single J-type shock model from Brand et al. (1988), are also displayed for comparison. We also checked the NY08 approximation as shown in Figure 6.4. Our best fit value is obtained at $b_{SE} = 3.2$ for $\chi = 0.6$. Again, this approach yields satisfying results for levels with a low excitation energy but tends to deviate at high excitation energy.

Finally, we extend our computation of $\chi^2$ until 44 rovibrational transitions, for which the vibrational levels $v$ varies from 0 to 4 (the upper limits are also discarded). The best comparison to observation ($\chi = 0.45$) is showed in Figure 6.4. The parameters
| Parameter | Value   | Description                   |
|-----------|---------|-------------------------------|
| $n_H$     | $10^4 \text{ cm}^{-3}$ | Pre-shock density of H nuclei |
| $b_0$     | $4.5 \pm 0.9$ | Strength of the magnetic field |
| $u_0$     | $\geq 30 \text{ km s}^{-1}$ | 3D terminal velocity |
| age       | $10^3 \text{ yr}$ | shock’s age                   |
| $\psi$    | $90^\circ \pm 30^\circ$ | Orientation of the magnetic field |
| $\beta$   | $2.1 \pm 0.2$ | Shock shape                   |

**Table 6.2:** Optimal parameters of the OMC-1 Peak1 (pure rotational levels) found with our model (see Figure 6.3).

**Orion Peak1**

**Figure 6.3:** Pure rotational H$_2$ excitation diagram observed in OMC-1 Peak1 (Rosenthal et al., 2000) compared with various models: our best-fit 3D-model of bow shock (open symbols), and the best fit models from Rosenthal et al. (2000): a combination of two planar C-shocks models from Kaufman and Neufeld (1996) (KN96) and one J-type shock model from Brand et al. (1988) (B88).
Figure 6.4: Same as Figure 6.3, with in addition the best-fitting power-law statistical equilibrium assumption models (see text). *yellow hexagons:* best fit with power-index $b_{SE} = 3.2$, while the other symbols are the same.

| Parameter | Value | Description |
|-----------|-------|-------------|
| $n_H$     | $10^6$ cm$^{-3}$ | Pre-shock density of H nuclei |
| $b_0$     | $3^{+2.5}_{-1.5}$ | Strength of the magnetic field |
| $u_0$     | $\geq 30$ km s$^{-1}$ | 3D terminal velocity |
| age       | $10^3$ yr | shock’s age |
| $\psi$    | $70^\circ \pm 25^\circ$ | Orientation of the magnetic field |
| $\beta$   | $2.4 \pm 0.27$ | Shock shape |

Table 6.3: Optimal parameters of the OMC-1 Peak1 (44 rovibrational levels) found with our model (see Figure 6.5).

that reproduce this best fit are listed in Table 6.3. The 3-$\sigma$ uncertainty range for some parameters is also provided.
6.2 $\text{H}_2$ line shape

The previous section 5.6 shows that a wealth of dynamical information is contained in the line shapes. However, this information is difficult to retrieve, as the line shaping process is quite convoluted. In particular, each line probes different regions of the shock depending on the upper level sensitivity to temperature.

6.2.1 HH54

We plot the normalized line shapes for three different transitions in a 20 km s$^{-1}$ bow shock with pre-shock density $10^4$ cm$^{-3}$, age 1000 yr and $b_0 = 1$ (Figure 6.6). This figure compares well with the figure 2 in Santangelo et al. (2014), which plots resolved observations of $\text{H}_2$ lines in HH54. These observations come from two different slit positions: a CRIRES slit for 1-0S(1) and 0-0S(9) near the tip of the bow, orthogonal to the outflow axis, and a VISIR slit for the 0-0S(4) line along this axis. On the other hand, our models cover the whole extent of our bow shock, which questions the validity of the comparison.
Figure 6.6: Line profiles of three different transitions in a bow shock at age 100 yr with parameters $u_0=20$ km s$^{-1}$, $n_H=10^4$ cm$^{-3}$, $b_0=1$, and viewing angle $i = -60^\circ$.

Despite this, some similarities are striking: the two lines 1-0S(1) and 0-0S(9) perfectly match and are blue-shifted. The insight from our computations allows us to link the good match between the line profiles of 1-0S(1) and 0-0S(9) to the very similar energy of the upper level of the two transitions. Furthermore, we checked that the emission from the low energy 0-0S(4) in our model is completely dominated by the C-type parts of our shocks, where the velocity is still close to the ambient medium velocity: this explains why this line peaks around $V_r = 0$. This C-type component should shine all over the working surface of the bow shock, and the VISIR slit along the axis probably samples it adequately. Conversely, we checked that the emission coming from lines 1-0S(1) and 0-0S(9) is completely dominated by the J-type parts of our shocks. Hence they should shine near the tip of the bow shock (traversed by the CRRES slit) at a velocity close to that of the star and its observed radial speed should lie around $-u_0 \cos(i)$, blue-shifted for an acute angle $i$.

6.2.2 Orion BN-KL outflow

Brand et al. (1989) managed to observe a few wide H$_2$ line profiles from OMC-1 Peak1 by using the UKIRT telescope, configured at a 5" sky aperture and with a resolution of 12 km s$^{-1}$ full width at half maximum (FWHM). A single shock model was not able to reproduce these wide observed lines (as indicated by Brand et al. 1989 and Rosenthal...
Figure 6.7: Comparison of the H$_2$ line profile between OMC-1 Peak1 observation and a bow shock model. **Black square:** the observational data (Brand et al., 1989). **Solid lines:** our 3D model using parameters in Table 6.2 with different values of $u_0$. The best 3D model constrains the terminal shock velocity to about 100 km s$^{-1}$.

et al. 2000). A C-type bow shock model of Smith et al. (1991b) could reproduce these lines and widths, but this assumed a extremely high magnetic field strength of $\gtrsim 50$ mG (which amounts to $b_\parallel \gtrsim 50$ for $n_H \sim 10^6$ cm$^{-3}$) while independent measurements in the same region gave much lower values: 3 mG by Zeeman splitting (Norris, 1984) or 10mG by polarization (Chrysostomou et al., 1994). Here we use the best parameters listed in Table 6.2 to try and reproduce the profile of the H$_2$ 1-0S(1) line with a more reasonable magnetization. As mentioned in the previous subsection, the excitation diagram alone did not allow to constrain the terminal shock velocity. Now, the width of the profile allows us to constrain the velocity to about $u_0 = 100$ km s$^{-1}$ as illustrated by Figure 6.7. The viewing angle $\beta \approx 90^\circ$ can be adjusted to the position of the peak of the line profile. Note that shock models with $u_\perp >40$ km s$^{-1}$ are not included in these line shape models. They should contribute little to the emission since H$_2$ molecules are dissociated at high shock velocities (both due to the high temperatures experienced in these shocks and to their radiative precursors).
Chapter 7

CONCLUSIONS AND PERSPECTIVES

7.1 Conclusions and remarks

In this study, we provide a mathematical formulation which links an arbitrarily shaped bow shock to a distribution of planar shocks. Then, a simple convolution of this distribution with a grid of planar shocks allows to produce intensities and line shapes for any transition of the H$_2$ molecule.

We used that property to explain the dependence of the excitation diagram of a bow shock to its parameters: terminal velocity, density, shape, age, and magnetization properties (magnitude and orientation). The combination of a steeply decreasing distribution with a threshold effect linked to the energy of the upper level of each transition yields a “Gamow-peak” effect. A given H$_2$ level then reaches a saturation value of column density when the terminal velocity is above a threshold which depends directly on the energy of the level. The magnetic field and the age dependence enter through the transition between the J-type and the C-type part of a time-dependent magnetized shock.

The wings of a bow shock usually have a larger surface than its nose. From this, it follows that the distribution and hence the global emission properties of a bow shock are generally dominated by low-velocity shocks. A direct consequence is that the excitation diagram of a whole bow shock resembles a 1D planar shock with a lower velocity: data interpretation with 1D models is likely to be biased towards low velocity. However, if the terminal velocity of the bow shock was estimated independently (from line Doppler broadening measurements, for example), we suggest that a magnetization adjustment from 1D models to the excitation diagram will over estimate the magnetization parameter. Previous authors
(NY08, Neufeld et al., 2009) have suggested that the statistical equilibrium approximation could accurately reproduce observed intensities of low-energy pure rotational levels. We confirm this result, and its probable link to the distribution of entrance velocities as pointed out by NY08. However, we remark that this simple model does not satisfyingly reproduce the observations of the higher-lying transitions. A possible interpretation is that these levels are more sensitive to J-type shocks, where the sudden temperature jump is more likely to put the gas away from statistical equilibrium.

We provide some illustrations of how our results could improve the match between model and observations in BHR71 and Orion OMC-1. We show that 3D models largely improve the interpretation. In particular, we are able to obtain much better match than in previous works with relatively little effort (and with the addition of only one or two parameters compared to the 1D models: the magnetic field orientation and the shape of the bow shock).

We compute line shapes with an unprecedented care and examine their dependence on age and viewing angle. Although line shapes result from a convoluted process, they contain a wealth of dynamical information. In particular, we link the double peaked structure of 1-0S(1) in young bow shocks to the dynamics of their J-type part components. The line width results from the combined effects of geometry, terminal velocity, and thermal Doppler effect. We show how different lines probe different parts of the shocks depending on the temperature sensitivity of the excitation of their upper level. We show how our 3D model can reproduce the broad velocity profile of the H$_2$ 1-0S(1) line in Orion Peak1 with a magnetization compatible with other measurements. The excitation diagram fails to recover dynamical information on the velocity (it only gives a minimum value), but the line shape width provides the missing constraint, which agrees with proper motion $\sim 100$ km s$^{-1}$ of the tips of the H$_2$ “fingers” in the region.

### 7.2 Perspectives

All models presented here were run for a pre-shock ortho-para ratio of 3 (Appendix A). However, the dilute ISM is known to experience much lower ratios and that should vary as a function of the excitation temperature (Neufeld et al., 2006). This variation is illustrated in Figure 7.1. David Neufeld suggested we should explore the effect of this parameter on the excitation diagrams of bow-shocks in future work and compare again to the observable data from shocks in BHR71 and OMC-1 Peak1 (chapter 6).

We have started to investigate a grid of models with a lower ortho/para ratio. For example, Figure 7.2 shows the comparison between BHR71 observations and the best bow shock model, for which the initial ortho/para ratio is 1. Due to the jagged variation of
the statistical weight of H₂ levels (which differ for even and odd rotational number $J$), the excitation diagram at low ortho-para ratios show a characteristic oscillation between ortho and para levels. Contrary to the one in Figure 6.1, the best fit diagram is not a smooth curve anymore and displays the similar weak oscillations as the observations. At low excitation energy, the fit is better than in the previous case with ortho/para=3, while it looks worse for higher excitation levels. We will investigate it further with David Neufeld and examine systematically the effect of the ortho-para ratio on 3D models of bow-shocks.

We are co-Is of two observational program with SOFIA-EXES, that will target pure rotational H₂ lines: S(1) and S(5)) in a sample of Galactic supernova remnants (IC443, W28, W44, 3C391), while S(4) and S(7) in a sample of molecular cloud (HH7). These observations will provide the first velocity resolved H₂ spectra in SNRs and in molecular cloud (velocity resolution of a few km s$^{-1}$). Our objective for those studies is to confront our models with H₂ spectra in simple geometries (spherical, in the case of IC443), in order to pinpoint the kind of shocks that are propagating in these environments (whether they are magnetized or not, stationary or not, dissociative or not), and to formulate diagnostics for their physical conditions.
Previous H₂ maps of 3D bow-shocks (Gustafsson et al., 2010) assumed that the direction of the flow was unperturbed (z-axis approximation). This is valid for C-type shocks, but not for J-type shocks. We plan to model both C-type and J-type shock trajectories by using a local planar approximation and to compare the resulting H₂ maps to previous work.

Our methods could be used to model other molecules of interest, provided that we know their excitation properties throughout the shock and that their emission remains optically thin. We expect that such developments will improve considerably the predictive and interpretative power of shock models in a number of astrophysical cases. In particular, if some excited CO lines can be assumed optically thin, they will allow direct probes of the dynamics of the gas. For the optically thick lines, one will need to be much more careful with the radiative transfer, but we could think using our method to build a 3D map with the correct CO abundance, and post-process it with a 3D radiative tool such as RADMC (Dullemond et al., 2012, or seelook at http://www.ita.uni-heidelberg.de/dullemond/software/radmc-3d/).

Further work will address some of the shortcomings of our method. First, it will be straightforward to apply similar techniques to the shocked stellar wind side of the bow shock working surface, helping us to access knowledge on the reverse shock (see chapter 9). Second, the different tangential velocities experienced on the outside and on the inner side of the working surface will very likely lead to Kelvin-Helmoltz instabilities,
generate turbulence and hence mixing, as multidimensional simulations of J-type bow
shocks show. A challenge of the simplified models such as the ones presented here will
be to include the mixing inside the working surface. One way of proceeding will be
to bracket the true behaviour between the two extreme situations. In the first situation,
the contact discontinuity between the two forward and reverse shocks remain stable, and
the observations can be simply modeled through the same methods presented here. In
the second situation, one can assume the fluid in between the two forward and reverse
shocks is completely mixed, just as Wilkin (1996) did for mass and momentum, but ex-
tending this property to energy and chemical composition. This will allow to compute
self-consistently the shape of the working surface, its chemical composition, temperature,
emission properties, etc... Note the same method can be utilized in the context of shocks
in binary winds, where we can expect to build powerful tools to synthesize observations
(see section 10.2).
Part III

STELLAR WIND MODEL
Chapter 8

GOVERNING EQUATIONS

The hydrodynamic model of the stellar wind from a AGB star is the solution of a set of hydrodynamic equations (subsection 4.1.1), associated with a chemical network. In order to achieve a set of simplified numerical equations of that system, we assume spherical symmetry of the central star and its circumstellar envelope. This assumption satisfies observations at least in the outer region of the circumstellar envelope (e.g., Figure 1.12), but is uncertain very close to the star. Observing the CO lines from AGB stars (e.g., RS Cancri and EP Aquarii, Mira Ceti, Red Rectangle), our collaborators \(^1\) found significant evidences for an asymmetric morphology close to the star. (e.g., Anh et al. 2015, Nhun et al. 2015b, Diep et al. 2016, Hoai et al. 2016)

8.1 Hydrodynamics

The velocity and density profiles of the circumstellar outflow are determined by the physical laws of mass conservation and momentum conservation. Throughout this work, we mostly consider an ideal fluid, so that the viscous and conducting phenomena are neglected, except in the case of a terminal wind shock, where we trigger a viscous jump. For the hydrodynamics of this gas, we consider a multicomponent fluid made of several gaseous chemical species and micron scale solid particles. Under these assumptions, the continuity equation of the gas can be derived from mass conservation as

\[
\frac{\partial \rho}{\partial t} + \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 \rho v) = 0 \tag{8.1}
\]

\(^1\)https://vnsc.org.vn/dap/
with $\rho$ the total mass density, $t$ the time, $r$ the radial coordinate, and $v$ the gas velocity. Note that the mass conservation equation for the neutrals is equivalent to Equation 4.3 with $z = r - r_0$ ($r_0$ is the starting radius of the computation) and $S_n \to S_n - 2\rho_n v_n/r$: the only additional contribution compared to the original planar mass conservation equation in the Paris-Durham shock code is geometrical dilution. Similarly, chemical equations have their source term transformed as $N_n \to N_n - 2n_n v_n/r$ for the neutrals and $N_i \to N_i - 2n_i v_i/r$ for the ions. The neutral momentum source has $A_n \to A_n - 2\rho_n v_n^2/r$ and the corresponding energy source has $B_n \to B_n - 2(\frac{1}{2} \rho v_n^2 + \frac{\gamma}{\gamma - 1} n_n k_B T_n) v_n/r$, etc... This is the convenient way we use to introduce geometrical dilution due to spherical geometry in the Paris-Durham planar shock code.

In the case of stationarity, Equation 8.1 can be integrated to yield

$$\dot{M} = 4\pi r^2 \rho v$$ \hspace{1cm} (8.2)

where the mass loss rate $\dot{M}$ is one of the fundamental model parameters and does not depend on the radius.

Similarly, the stationary equation of motion in spherical symmetry is derived from the law of momentum conservation

$$v \frac{\partial v}{\partial r} = \frac{1}{\rho} f - \frac{1}{\rho} \frac{\partial P}{\partial r}$$ \hspace{1cm} (8.3)

with $f$ the algebraic sum of the external forces acting on a unit volume and $P$ the internal gas pressure. Once dust-grains form, the radiation force from the star acting on the dust particles accelerates them outward. The surrounding gas particles then will be dragged along by collisions with the dust. Therefore, the external force $f = f_{\text{grav}} + f_{\text{drag}}$. Gravitation force ($f_{\text{grav}}$) attracts the gas inward to the stellar center, while drag force ($f_{\text{drag}}$) drives it outward.

The gravitation force per a unit volume is simply proportional to $r^{-2}$

$$f_{\text{grav}} = -G \frac{M_* \rho}{r^2}$$ \hspace{1cm} (8.4)

The drag force, on the other hand, is somewhat more complicated. This force depends on the relative drift speed, $v_{\text{drift}}$, between the gas and dust components

$$v_{\text{drift}} = v_d - v$$ \hspace{1cm} (8.5)
where \( v_d \) is the flow speed of the dust and \( v_d > v \). There are two expressions for the drag force depending on the thermal sound speed of gas

\[
c_s = \sqrt{\frac{P}{\rho}} = \sqrt{\frac{\gamma k_B T}{\mu m_H}} \tag{8.6}
\]

where \( \gamma \) is the ratio the specific heats, \( \mu \) is molecular weight of gas and \( m_H \) is the mass of a proton. Depending on the composition of the gas, its molecular weight can be different. For example, \( \mu \approx 2.33 \) for a mixture between helium and molecular hydrogen, while a mixture with atomic hydrogen has \( \mu \approx 1.4 \).

If the drift speed is much faster than the thermal sound speed of the gas particles, the ram pressure acting on the gas is \( \rho v_d^2 \); and the drag force per unit volume of gas, therefore, is the product of that ram pressure times the cross-section of the dust grain:

\[
f_{\text{drag}}(a) = \pi a^2 n_g \rho v_d^2 \tag{8.7}
\]

To combine two those limits, we can express the drag force as below

\[
f_{\text{drag}}(a) = \pi a^2 n_g \rho v_d^2 \sqrt{v_d^2 + c_s^2} \tag{8.7}
\]

Since the mean free path of the gas is higher than the typical dust radii and the velocities of gas and dust are different from each other, the grains are not position coupled to the gas. Despite the fact that the grains collide with only a small fraction of the gas particles, Gilman (1972) indicates that the subsequent collisions among the gas molecules allow the momentum that they receive from the radiation field to be transferred to the gas. Gilman (1972) also demonstrates that the small grains rapidly reach the terminal drift velocity. The grains move at the terminal drift velocity when the radiation force balances with the drag force:

\[
f_{\text{drag}} = f_{\text{rad}} \tag{8.8}
\]

where \( n_d \) is the dust number density and \( f_{\text{rad}} \) is the radiation force acting on one grain, defined by

\[
f_{\text{rad}} = \frac{\sigma_d Q_{rp} L_\star}{4\pi c_l^2} \tag{8.9}
\]

where \( \sigma_d = \pi a^2 \) is the grain cross-section (assumed circular here) and \( c_l \) is the speed of light. \( Q_{rp} \) is the radiation pressure efficiency and \( Q_{\star \text{rp}} \) is the wavelength averaged radiation pressure efficiency weighted by the stellar spectrum. \( L_\star \) is the total stellar luminosity. It is determined through the absorption \( Q_{\text{ext}}(a, \lambda) \) and scattering \( Q_{\text{sca}}(a, \lambda) \) coefficients which are calculated by using the Mie theory with complex radiative indices (subsection 8.3.1).
Let us assume that the grains are moving at terminal drift velocity, the momentum Equation 8.3 now expands as

\[ \frac{v}{r} \frac{\partial v}{\partial r} + \frac{1}{\rho} \frac{\partial P}{\partial r} = -\frac{GM_s}{r^2} + n_d \frac{\sigma_d Q_{rp} L_s}{4 \pi r^2 c_l} \]  

(8.10)

The two terms on the right hand side in Equation 8.10 vary as \( r^{-2} \), it is hence convenient to group them in a simple form of the momentum equation

\[ \frac{v}{r} \frac{\partial v}{\partial r} + \frac{1}{\rho} \frac{\partial P}{\partial r} = (\Gamma - 1) \frac{GM_s}{r^2} \]  

(8.11)

with the radiative acceleration on one spherical species of dust

\[ \Gamma(a) = n_d \frac{\sigma_d Q_{rp}(a)L_s}{4 \pi c_l GM_s \rho} \]  

(8.12)

Equation 8.11 can be rewritten in the form of the standard wind equation

\[ \left( \frac{v^2 - c_s^2}{v} \right) \frac{\partial v}{\partial r} = 2c_s^2 \frac{1}{r} - \frac{\partial c_s^2}{\partial r} + (\Gamma - 1) \frac{GM_s}{r^2} \]  

(8.13)

with \( c_s^2 = P/\rho \). When the temperature profile (hence the isothermal sound speed profile) is prescribed, this equation shows the existence of a critical point at \( r = r_{ci} \), where the speed of the gas reaches the isothermal sound speed. That point is called the isothermal sonic point.

In the more realistic case where the temperature evolution is solved along the wind, we can also get an expression for the velocity gradient by combining mass, momentum and energy conservation so as to eliminate the pressure gradients. We arrive at

\[ \frac{\partial v}{\partial r} = \frac{1}{2} \frac{\gamma + 1}{\gamma - 1} S_n v^2 - \frac{\gamma}{\gamma - 1} A_n v + B_n \]  

\[ \frac{\gamma}{\gamma - 1} P - \frac{1}{\gamma - 1} \rho v^2 \]  

(8.14)

which is expressed after some simplifications as

\[ \left( \frac{v^2 - c_s^2}{v} \right) \frac{\partial v}{\partial r} = \frac{2v^2}{r} + (\Gamma - 1) \frac{GM_s}{r^2} + (\gamma - 1) \frac{\Lambda}{\rho v} \]  

(8.15)

where \( \Lambda \) is the net radiative cooling. This last form closely resembles Equation 8.13 and applies in the general case. It shows that the sonic point when cooling and heating are introduced occurs when the velocity crosses the adiabatic sound speed.
However, we experienced numerical issues when integrating Equation 8.15, and we were never able to cross the sonic point with this form. We found a compromise by using Equation 8.13 with $c_s$ in place of $c_i$ for the space derivative of the velocity from the stellar surface to the adiabatic sonic point $r = r_c$. We revert to the more proper Equation 8.15 after the sonic point has been crossed. The standard temperature gradient is used throughout to control the temperature profile.

Once the grains form, the thermal sound speed and its radial derivative are small compared to the last term on the right hand side of Equation 8.13. Therefore, the sonic point occurs at a radius just before the point where $\Gamma$ starts to be greater than unity.

We now consider a collection of spherical grain particles, with a constant size distribution $dn_d = f(a)da$. The resulting equivalent $\bar{\Gamma}$ of the radiative acceleration on dust is obtained through the relation

$$\bar{\Gamma} = \int \frac{\Gamma(a) f(a)}{n_d} da$$

(8.16)

where $n_d = \int da f(a)$ is the total density of grain particles, we adopt a standard spectrum of grain-size distribution $f(a) = Aa^b n_H$. For the interstellar dust, the spectral index $b$ is usually assumed to be equal to -3.5 from the famous MRN law (Mathis et al. 1977). For the circumstellar dust shell, (Dominik et al., 1989) deduced a steeper slope for the spectral distribution and estimated the spectral index $b \sim -5$. However, Decin et al. (2006) suggest that the choice of the slope has little influence on the resulting dynamics. Thus, we consider the term $A$, which is the factor giving the number of dust particles per $H$ atom, to be a constant for the case of the interstellar dust. Its value is estimated to be $10^{-25.10} \text{ cm}^{2.5}/H$ for Silicate grains and $10^{-25.13} \text{ cm}^{2.5}/H$ for carbon grains with size minimum and maximum boundaries $a_{\text{min}} = 0.005 \mu m$ and $a_{\text{max}} = 0.25 \mu m$ (Draine and Lee 1984).

## 8.2 Thermodynamics

The temperature profile of the multicomponent outflow circumstellar envelope, consisting of gas molecules and solid grain particles, is determined by the laws of thermodynamics. The gas molecules are assumed to be characterized by their local kinetic temperature $T(r)$. Each grain particle characterized by its radius $a$ is also assumed to be a thermal emitter, characterized by the size-dependent temperature $T_d(a, r)$. 
8.2.1 Gas temperature

In this section, we describe only the cooling and heating terms specific to the stellar wind situation. The standard heating and cooling terms of the Paris-Durham shock code as described in chapter 4 still apply and are considered in our wind models.

8.2.1.1 Grain-gas collisional heating

As mentioned in section 8.1, the grains rapidly reach their terminal drift velocity. They move at the terminal velocity if the drag force balances with the radiation force. The balance of these terms for grain of size $a$ leads to

$$\frac{\dot{Q}_{\text{rp}}(a) L_*}{4\pi r^2 c_l} = \rho v_{\text{drift}} \sqrt{v_{\text{drift}}^2(a) + c_s^2}$$

(8.17)

The expression for the drift velocity is derived by taking the square at both sides of Equation 8.17

$$v_{\text{drift}}^4(a) + c_s^2 v_{\text{drift}}^2(a) - \left(\frac{\dot{Q}_{\text{rp}}(a) L_*}{4\pi r^2 \rho c_l}\right)^2 = 0.$$  

(8.18)

Solving the second order Equation 8.18 in $v_{\text{drift}}$ and combining the solution with Equation 8.2 give

$$v_{\text{drift}}(a) = \frac{1}{2} \left[ \left( \frac{2v}{M c_l} \dot{Q}_{\text{rp}}(a) L_* \right)^2 + c_s^4 \right]^{0.5} - c_s^2$$

(8.19)

In the limiting case where the sound speed $c_s$ is small compared to the outflow speed $v$, this expression reduces to

$$v_{\text{drift}}(a) = \sqrt{\frac{\dot{Q}_{\text{rp}}(a) L_* v}{M c_l}}.$$  

(8.20)

This expression for the drift velocity shows the dependence on the mass-loss rate $\dot{M}$ and the outflow speed $v$. The gas-grain collisions, therefore, become increasingly important as the distance from the star increases and $v$ reaches its terminal value. The resulting heating rate corresponds to the work done by the drag force. For the whole distribution of grains, this yields:

$$q_{\text{drift}} = \rho \int da f(a)^{\frac{1}{2}} \sigma_d v_{\text{drift}}^3(a).$$

(8.21)
8.2.1.2 Molecular pumping from stellar radiation

Close to the star, the molecular gas receives energy from the radiation field that is able to excite the molecules into higher excitation levels. Then, molecules cool down by spontaneous de-excitation processes, or by collisional de-excitation, in which case the radiation energy is transferred to the gas as thermal energy. In this section, we study the pumping effect from the stellar radiation to molecules.

Let’s consider a system of two levels, with \( n_i \) and \( n_j \) column densities of the upper and lower levels, respectively. The corresponding energies are \( E_i \) and \( E_j \), where \( \Delta E = E_i - E_j = h\nu_{ij} \). The number of density of atoms in the level \( i \) changes basically due to: (1) spontaneous emission, (2) stimulated emission, (3) photon absorption, and (4) collisions. This variation per unit time is defined as:

\[
\frac{dn_i}{dt} = -n_i \left[ A_{ij} + B_{ij} \rho(\nu_{ij}) + C_{ij} \right] + n_j \left[ B_{ji} \rho(\nu_{ij}) + C_{ji} \right] \tag{8.22}
\]

where \( \rho(\nu) \) is the spectral energy density at frequency \( \nu \) of the radiation field and \( T_{ij} = \Delta E/k_B \). If we consider the star as a black-body, \( \rho(\nu_{ij}) \) is defined by Planck’s law as:

\[
\rho(\nu_{ij}) = \frac{1}{4} \left( \frac{R_*}{r} \right)^2 \frac{F(\nu_{ij})}{e^{T_{ij}/T_*} - 1} \tag{8.23}
\]

with \( R_* \) the stellar radius, and \( F(\nu_{ij}) \) a function defined as

\[
F(\nu_{ij}) = \frac{8\pi h\nu_{ij}^3}{c^3} \tag{8.24}
\]

where \( A_{ij}, B_{ij}, B_{ji} \) are the Einstein coefficients. \( A_{ij} \) is the probability in unit time that a particle in state \( i \) spontaneously decays to the stage \( j \). \( B_{ij} \) is the probability per unit time per unit spectral energy density of the radiation field that a particle in the stage \( i \) decays by stimulation to the stage \( j \). \( B_{ji} \) is the probability per unit time per unit spectral energy density of the radiation field that a particle in state \( j \) absorbs a photon to jump to state \( i \). \( C_{ij} \) and \( C_{ji} \) are the collisional de-excitation and excitation coefficients. These coefficients are linked with each other by

\[
A_{ij} = F(\nu_{ij})B_{ij} \tag{8.25}
\]

\[
B_{ij} = \frac{g_j}{g_i} B_{ji} \tag{8.26}
\]

\[
C_{ij} = \frac{n}{n_{C_{ij}}} A_{ij} \tag{8.27}
\]
with \( n \) the total density of colliders, \( n_{C_{ij}} \) the critical density of the transition, and \( T \) the gas temperature. We can rewrite Equation 8.22 in a simple form

\[
\frac{dn_i}{dt} = -n_i(A_{ij} + C_{ij}) + (n_j B_{ji} - n_i B_{ij}) \rho(\nu_{ij}) + n_j C_{ji} \tag{8.29}
\]

Substituting those expressions into Equation 8.29, while keeping \( A_{ij} \) as a reference coefficient, we have:

\[
\frac{dn_i}{dt} = -n_i \left( A_{ij} + \frac{n}{n_{C_{ij}}} \right) + n_j \left( A_{ij} \frac{g_i}{g_j} e^{-T_{ij}/T_{kin}} \right) + \frac{A_{ij}}{F(\nu)} \left( n_j \frac{g_i}{g_j} - n_i \right) \frac{1}{4} \left( \frac{R_*}{r} \right)^2 \frac{F(\nu)}{e^{T_{ij}/T_*} - 1} + n_j \frac{g_i}{g_j} \left( -n_j + n_j \frac{g_i}{g_j} e^{-T_{ij}/T_{kin}} \right) + \frac{n_j g_i}{g_j} - \frac{n_i}{g_j} 1 \frac{1}{4} \left( \frac{R_*}{r} \right)^2
\]

\[
= A_{ij} \left[ -n_i + \frac{n}{n_{C_{ij}}} \left( -n_i + n_j \frac{g_i}{g_j} e^{-T_{ij}/T_{kin}} \right) + \frac{n_j g_i}{g_j} - \frac{n_i}{g_j} \right] \frac{1}{4} \left( \frac{R_*}{r} \right)^2 \tag{8.30}
\]

In thermodynamic equilibrium, the density \( n_i \) (\( n_j \)) is proportional to the product between the statistical weight \( g_i \) (\( g_j \)) and the Boltzmann factor at the temperature \( T \):

\[
n_i = n_M \frac{g_i}{Z} e^{-T_i/T_{ex}}
\]

\[
n_j = n_M \frac{g_j}{Z} e^{-T_j/T_{ex}} \tag{8.31}
\]

\[
\frac{n_j}{n_i} = \frac{g_j}{g_i} e^{(T_i - T_j)/T_{ex}} = \frac{g_j}{g_i} e^{T_{ij}/T_{ex}}
\]

with \( n_M \) the density of the molecule considered and \( Z(T) = \sum_i g_i e^{-T_i/T} \) the partition function. At high density we are close to steady-state and \( dn_i/dt = 0 \). Thus, the net rate
of energy lose for the gas through collisions is then:

\[ \Lambda_i = h \nu_{ij} (n_j C_{ji} - n_i C_{ij}) \]
\[ = A_{ij} n_i \left( -n_i + n_j \frac{g_i}{g_j} e^{-T_{ij}/T_{kin}} \right) \]
\[ = A_{ij} \nu_{ij} \left[ -n_i + \frac{\frac{g_i}{g_j} - n_i}{e^{T_{ij}/T_*} - 1} \left( \frac{R_*}{r} \right)^2 \frac{1}{4} \right] \]
\[ = -A_{ij} n_i \nu_{ij} \left[ 1 - e^{T_{ij}/T_{ex}} - 1 \left( \frac{R_*}{r} \right)^2 \frac{1}{4} \right]. \] (8.32)

As long as the local thermal equilibrium (LTE) is satisfied, \( T_{kin} = T_{ex} = T \). Then the rate of energy lose is:

\[ \Lambda_i = -A_{ij} n_i \nu_{ij} \left[ 1 - e^{T_{ij}/T_{ex}} - 1 \left( \frac{R_*}{r} \right)^2 \frac{1}{4} \right]. \] (8.33)

If \( T, T_* \ll T_{ij} \), one might replace \( e^{T_{ij}/T} - 1 \) and \( e^{T_{ij}/T_*} - 1 \) by \( e^{T_{ij}/T} \) and \( e^{T_{ij}/T_*} \), \( \Lambda_i \) approximates to

\[ \Lambda_i = -A_{ij} n_i \nu_{ij} \left[ 1 - \frac{1}{4} \left( \frac{R_*}{r} \right)^2 e^{T_{ij}(\frac{T}{T_*} - \frac{1}{T_*})} \right]. \] (8.34)

If \( T, T_* \gg T_{ij} \), one might replace \( e^{T_{ij}/T} \) and \( \exp(T_{ij}/T_*) \) by \( 1 + T_{ij}/T \) and \( 1 + T_{ij}/T_* \), \( \Lambda_i \) approximates to

\[ \Lambda_i = -A_{ij} n_i \nu_{ij} \left[ 1 - \frac{T_*}{4} \frac{T}{T_*} \left( \frac{R_*}{r} \right)^2 \right]. \] (8.35)

This last case is valid next to the star where the temperature is high compared to the typical transition energies of the molecules. Note that \( -A_{ij} n_i \nu_{ij} \) in unit of \( \text{erg cm}^{-3} \text{s}^{-1} \) is the cooling term, which is already embedded into the Paris-Durham shock code (chapter 4). Therefore, close to the star, where LTE applies, the pumping of molecules by the stellar radiation field can be considered simply by multiplying by a factor of \( \left[ 1 - (1/4) (T_*/T) (R_*/r)^2 \right] \) the molecular cooling term. Far from the star, this factor is close to 1 and the standard ISM non-LTE cooling functions apply.
8.2.2 Grain temperature and condensation radius

The grain temperature evolution is determined by a balance between the heating and the cooling rate. In principle, the grains can be heated either by collisions with the gas particles or by direct absorption of stellar or ambient radiation. The grains also can be cooled either by collisional energy transfer or by thermal radiation. We assume here that the stellar radiation dominates. The balance that determines the grain temperature \( T_d \), henceforth, is based on the radiative equilibrium condition

\[
\int_{0}^{\infty} k_\lambda B_\lambda(T_d)d\lambda = \int_{0}^{\infty} k_\lambda J_\lambda d\lambda
\]  

(8.36)

with \( k_\lambda \) the opacity related to the cross-section of a grain \( \sigma Q_{\text{abs}}(a, \lambda) \). The left hand side of Equation 8.36 is the radiative cooling of a grain assumed to be a black-body at wavelength \( \lambda \) and temperature \( T_d \). The right hand side of Equation 8.36 is the radiative heating from the monochromatic mean intensity \( J_\lambda \) of the stellar radiation field, for which the average of the radiation intensity \( I_\lambda \) is

\[
J_\lambda = \frac{1}{4\pi} \int_{0}^{4\pi} I_\lambda d\Omega.
\]  

(8.37)

Far from to the star, the radiation is well approximated by a diluted Black-body radiation:

\[
J_\lambda = W(r) B_\lambda(T_*)
\]  

(8.38)

where \( W(r) \sim \frac{1}{4}(R_*/r)^2 \) is the geometrical dilution factor.

The radiation condition from Equation 8.36 for a grain is expanded to

\[
\int_{0}^{\infty} \pi a^2 Q_{\text{abs}}(a, T_d) B_\lambda(T_d)d\lambda = \int_{0}^{\infty} \pi a^2 Q_{\text{abs}}(a, T_*) B_\lambda(T_*) W(r)d\lambda.
\]  

(8.39)

Dividing both sides of Equation 8.39 by \( \int_{0}^{\infty} B_\lambda(T) \), the left and right integrations are simply reformulated as the Planck mean efficiency \( Q_{\text{abs}}^P(a, T) \). Therefore, the grain temperature is a function of the radius \( r \), which satisfies the relation

\[
T_d^4 Q_{\text{abs}}^P(a, T_d) = T_*^4 W(r) Q_{\text{abs}}^P(a, T_*) \quad \text{or}
\]

\[
T_d = T_* W^{1/4} \left\{ \frac{Q_P(a, T_*)}{Q_P(a, T_d)} \right\}^{1/4}
\]  

(8.40)
Chapter 8. Basic equations

Close to the star, the geometrical dilution factor $W$ equals $1/2$ and Equation 8.40 indicates that the grain temperature is almost as high as the stellar temperature. In fact, at such high temperature, the grains can not exist because of sublimation. However, we can find the innermost distance $r_c$ where the grains may form by replacing the grain temperature $T_d$ by the grain condensation temperature $T_c$ in the Equation 8.36. In the simple case when the grain absorption efficiency can be approximated as a power-law of wavelength ($Q_{abs} \approx \lambda^{-p}$), the innermost distance $r_c$ is determined as

$$r_c = \frac{R_*}{2} \left( \frac{T_*}{T_c} \right)^{\frac{4+p}{p}}. \quad (8.41)$$

8.3 Interaction between grain particles and stellar radiation

8.3.1 Mie theory for spherical grains

As shown in Equation 8.9, in order to calculate the radiative acceleration on dust $\bar{\Gamma}$, the quantity of the radiation pressure coefficient $Q_{rp}$ is required.

The radiation pressure coefficient is given by

$$Q_{rp}(a, \lambda) = Q_{abs}(a, \lambda) + (1 - g)Q_{sca}(a, \lambda) \quad (8.42)$$

where $Q_{abs}$, $Q_{sca}$ and $g$ are the absorption coefficient, scattering coefficient and anisotropy parameter. In the case of perfect forward-scattering $Q_{rp} = Q_{abs}$, isotropy scattering $Q_{rp} = Q_{abs} + Q_{sca} = Q_{ext}$ and perfect back-scattering $Q_{rp} = Q_{abs} + 2Q_{sca}$. In the more general case of scattering, the anisotropy parameter has to be in between $\pm 1$.

The absorption and scattering coefficients are calculated by solving the appropriate boundary-value problem for Maxwell’s equation, which is known as the Mie theory (more detail can be found in Gail and Sedlmayr 2013). The result for those coefficients from Mie theory are given by the expression

$$Q_{ext} = \frac{2}{\pi^2} \sum_{j=1}^{\infty} (2j + 1) \text{Re}(a_j + b_j) \quad (8.43)$$

$$Q_{sca} = \frac{2}{\pi^2} \sum_{j=1}^{\infty} (2j + 1) \left(|a_j|^2 + |b_j|^2\right) \quad (8.44)$$

$$Q_{ext} = Q_{abs} + Q_{sca}. \quad (8.45)$$
The quantity $x$ is defined as

$$x = \frac{2\pi an_m}{\lambda} \tag{8.46}$$

where $\lambda/n_m$ represents the wavelength in a surrounding medium of refractive index $n_m$ where the dust is embedded. In the vacuum $n_m$ equals 1.

The coefficients $a_j$ and $b_j$ are defined by

$$a_j = \frac{m\psi_j(mx)\psi_j'(x) - \psi_j(x)\psi_j'(mx)}{m\psi_j(mx)\xi_j'(x) - \xi_j(x)\psi_j'(mx)}, \tag{8.47}$$

$$b_j = \frac{\psi_j(mx)\psi_j'(x) - m\psi_j(x)\psi_j'(mx)}{\psi_j(mx)\xi_j'(x) - m\xi_j(x)\psi_j'(mx)}.$$ 

The quantity $m = n^d/n_m$ is the ratio between the complex indices of refraction of the dust material $n^d$ and the surrounding. $n^d$ depends on the optical properties of each grain (see subsection 8.3.2).

The wave functions $\psi$ and $\xi$ are determined by the recurrence relation

$$\psi_{j+1}(x) = \frac{2j + 1}{x} \psi_j(x) - \psi_{j-1}(x) \tag{8.48}$$

$$\xi_{j+1}(x) = \frac{2j + 1}{x} \xi_j(x) - \xi_{j-1}(x).$$

The calculations start with

$$\psi_{-1}(x) = \cos x, \quad \psi_0(x) = \sin x$$

$$\xi_{-1}(x) = \cos x + i \sin x, \quad \xi_0(x) = \sin x - i \cos x. \tag{8.49}$$

### 8.3.2 Optical constants of dust materials

In order to construct the optical properties of grains and calculate the radiation pressure on the dust grains, the complex indices of refraction of the grain materials should be known. Although they are called optical 'constants', they are wavelength dependent and they vary depending on the grain type. They cannot be straightforwardly determined from observations. But they can be measured in the laboratory. The comparison between laboratory spectra and IR spectra from circumstellar shells (e.g., Figure 8.2) hence allows us to derive the possible features of grains. According to the elemental composition of
the stars and the thermal stability of condensed states, the grain material can be identified. The selection of grain material consistent with the stellar material composition (C/O ratio) is essential (see subsection 3.2.2). The first classification of grain material was studied by Gilman (1969) and Woolf and Ney (1969) by using the earliest IR spectra in circumstellar envelopes. Table 8.1 presents some dust species representative of oxygen-rich and carbon-rich stars. Based on their weak emission in the IR spectra (Figure 8.2), stars from the transition region between those two types (hereafter called S stars) can be considered as oxygen-rich stars.
Figure 8.2: Examples of IR spectra from circumstellar dust shells, which represent the main different types of AGB stars forming dust shells at different stages of their evolution: o Ceti (M-type), $\pi^1$ Gru (S-type) and RScl (C-type); PZ Cas is a super-giant with an M type spectrum (Gail and Sedlmayr, 2013).
Table 8.2: Initial elemental composition of the most abundant species in the solar photosphere when C/O equals 1.5 (Lodders et al. 2009). Numbers in parentheses are powers of 10.

| Element | Composition | Initial density \( (n/n_{\text{H}}) \) | Formation enthalpy |
|---------|-------------|----------------------------------------|-------------------|
| H       | 0100000000000000 | 1                                      | 51.634            |
| He      | 0000000100000000 | 8.414(-02)                             | 0.0000            |
| C       | 0005000000000000 | 2.455(-04)                             | 169.98            |
| N       | 0000100000000000 | 7.244(-05)                             | 112.53            |
| O       | 0000010000000000 | 2.455(-04)                             | 58.980            |
| Mg      | 0000000001000000 | 3.467(-05)                             | 35.000            |
| Si      | 0000000000100000 | 3.311(-05)                             | 106.70            |
| S       | 0000000000100000 | 1.380(-05)                             | 65.600            |
| Fe      | 0000000000010000 | 2.818(-05)                             | 98.700            |

8.4 Chemistry

8.4.1 Initial photospheric elemental compositions

Along the stellar wind, the evolution of chemical species essentially depends on the initial elemental composition at the stellar photosphere. We assume the elemental photospheric abundance to be the same as the solar abundance except for the C/O ratio. Each value of this ratio corresponds to an AGB type (Cherchneff 2006). Carbon-rich stars have C/O larger than 1 and on the contrary oxygen-rich stars have C/O lower than 1.

Most of the elemental abundances at the solar photosphere are deduced by spectroscopy: the emitted spectra are first calculated by atmospheric models; then calculated spectra are compared to the observed spectrum; and finally the abundances are returned based on those comparisons. However, the conversion from the spectrum to the value of abundances requires the theoretical knowledge of line position, transition probability and lifetime of excited levels. The local thermal equilibrium (LTE) for which excited levels are populated regarding the relations of Boltzmann and Saha is therefore usually used to calculate solar abundances. Table 8.2 shows most of the initial element compositions at the solar photosphere (Lodders et al. 2009).

8.4.2 Chemical network

In this study, we use the network from the Paris-Durham code (subsection 4.2.2), but we will focus on hydrogen chemistry. The Paris-Durham chemical network is optimized and includes most of the recent bimolecular reactions relevant for the interstellar
medium (Appendix G). However, the gas density in the inner envelope is sufficiently high \( n \gtrsim 10^{10} \text{ cm}^{-3} \) that the trimolecular processes can be initiated. Through those reactions, which matter for hydrogen, two atomic hydrogens react together, when another atomic hydrogen or a molecular hydrogen acts as a third body to evacuate the binding energy of the \( \text{H}_2 \) molecule

\[
\text{H} + \text{H}_2 \xrightleftharpoons[k_2]{k_3} \text{H} + \text{H} + \text{H}
\]

\[
\text{H}_2 + \text{H}_2 \xrightleftharpoons[k_4]{k_3} \text{H} + \text{H} + \text{H}_2.
\]

In a such dense medium, molecular hydrogen is formed by three-body recombination of hydrogen with rate coefficients \( k_2 \) and \( k_4 \), while it is destroyed by the collisional dissociation with rate coefficients \( k_1 \) and \( k_3 \). The values of those coefficients are discussed in the next section.

Finally, the formation of dust grains is not treated self-consistently throughout the model. Dust grains are turned on whenever the gas temperature is below the condensation temperature and then they remain constant. Thus, we turn off gas-grain reactions in the chemical network, except for the formation of \( \text{H}_2 \) at the grains’ surface.

### 8.4.3 Formulation of hydrogen chemistry on the stellar surface

#### 8.4.3.1 Discussion of selected reaction rate coefficients

The evolution of the abundance of molecular hydrogen \( x_2 = n(\text{H}_2)/n_{\text{H}} \) is generally expressed in the Lagrangian form (Glassgold and Huggins 1983) as:

\[
\frac{dx_2}{dt} = P - D x_2
\]

where \( P \) and \( D \) are the production and destruction rates of \( \text{H}_2 \). When it reaches equilibrium, these two rates must be equal. In chemical equilibrium, thus, the forward and backward rates in Equation 8.50 balance:

\[
n(\text{H})n(\text{H}_2)k_1 = n^3(\text{H})k_2
\]

and the Saha relation gives

\[
\frac{n(\text{H}_2)}{n^2(\text{H})} = \frac{Z(\text{H}_2)}{Z(\text{H})^2} \left( \frac{\hbar^2}{\pi m_{\text{H}} k_B T} \right)^{3/2} e^{\frac{E_{\text{diss}}}{k_B T}} = \frac{k_2}{k_1}
\]

(8.54)
where $E_{diss} = 4.48\text{eV}$ is the dissociation energy of $\text{H}_2$. The partition function of $\text{H}$ is $Z(H) = 2$ (Flower and Harris, 2007) or $Z(H) = 4$ if discernibility and electron degeneracy is taken into account (Forrey, 2013). The partition function of $\text{H}_2$ is defined by

$$Z(H_2) = \sum_i g_i e^{-\frac{E_i}{k_B T}}$$ (8.55)

where $g_i$ and $E_i$ are the statistical weight and energy for the excitation level $i$. According to the table of the excitation energy (Appendix F), Flower and Harris (2007) fit the partition $Z(H_2)$ as a function of temperature up to $\sim 2000 \text{K}$. The best fit gives the formula

$$Z(H_2) \simeq 0.028 T^{0.985}.$$ (8.56)

Knowing the rate coefficient $k_1$ allows us to derive the rate coefficient $k_2$. Figure 8.3 shows a few rate coefficients of $\text{H}_2$ collisional dissociation. The evolution of this rate coefficient with respect to the temperature differs between laboratory experiments (e.g., Jacobs et al. 1967, Breshears & Bird 1973 cited by Lepp and Shull 1983) and theoretical studies (e.g., Lepp and Shull 1983, Martin et al. 1996), and even with the UMIST database (Figure 8.3, top, this coefficient in UMIST has no precise reference cited but "literature search"). As many previous authors, we used the experimental rate coefficient from Jacobs et al. (1967). However, the latter is not the same in different citations as shown in the bottom of Figure 8.3. We chose

$$k_1 = 1.38 \times 10^{-4} T^{-1.025} e^{(-52000/T)}$$ (8.57)

in unit of $\text{cm}^3 \text{s}^{-1}$ (Jacobs et al. 1967; Flower and Harris 2007). Then Equation 8.54 allows us to derive

$$k_2 = 1.44 \times 10^{-26} T^{-1.54}$$ (8.58)

in unit of $\text{cm}^6 \text{s}^{-1}$. This derived rate coefficient, however, differs from Jacobs et al. (1967)’s deduced coefficient as

$$k_{2,J} = 5.52 \times 10^{-29} T^{-1}$$ (8.59)

and from the theoretical study of Forrey (2013)

$$k_{2,F} = 6 \times 10^{-32} T^{-1/4} + 2 \times 10^{-31} T^{-1/2}$$ (8.60)

in the same unit. Figure 8.4 illustrates the discrepancy between those three rate coefficients. In this work, we have chosen the rate coefficient of the recombination of three atomic hydrogen ($k_2$) as in Equation 8.58.
Figure 8.3: Studies of H-H₂ collisional dissociation rate coefficients. (Top) Discrepancy of collisional dissociation rate coefficients between experiments and theoretical studies. (Bottom) Discrepancy between citations of Jacobs et al. (1967)’s collisional dissociation rate coefficient.
The connection of the rate coefficients between Equation 8.50 and Equation 8.51 is

\[ \frac{k_1}{k_2} = \frac{k_3}{k_4} \]  

(8.61)

In practice, the rate coefficient \( k_4 \) (or \( k_3 \)) in Equation 8.51 is easier to measure in the laboratory than the rate coefficient \( k_2 \) (or \( k_1 \)) in Equation 8.50. Ham et al. (1970) and Cohen and Westberg (1983) made experiments at low temperature (up to room temperature \( \sim 300 \) K) to measure \( k_4 \), for which hydrogen is initially mainly molecular. Cohen and Westberg (1983) extrapolated it for high temperature and recommended the relation

\[ k_{4,C} = 2.8 \times 10^{-31} T^{-0.6} \]  

(8.62)

in unit of cm\(^6\) s\(^{-1}\). In addition, Jacobs et al. (1967) showed that this rate coefficient related to the rate coefficient \( k_2 \) as \( k_4 = k_2/8 \), and adopting Equation 8.58 for \( k_2 \), we get

\[ k_4 = k_2/8 = 1.8 \times 10^{-27} T^{-1.54} \]  

(8.63)

in the same units. Nevertheless, these two rate coefficients differ between each other by
a factor of 10 at 1000 K. That is \( k_{4C} \approx 4.4 \times 10^{-33} \text{ cm}^6 \text{ s}^{-1} \), while \( k_4 \approx 4.1 \times 10^{-32} \text{ cm}^6 \text{ s}^{-1} \) at \( T = 1000 \text{ K} \). Even so, in this work, we have chosen the rate coefficient \( k_4 \) (Equation 8.63). This choice bases on two reasons, which have been discussed by Flower and Harris (2007). First, the extrapolation of Cohen and Westberg (1983) to higher temperature remains uncertain; and second, the inverse reaction in Equation 8.50 is less important than in Equation 8.51 since atomic hydrogen is initially dominant at stellar surface, which is the opposite to the laboratory situation. Finally, the last rate coefficient \( (k_3) \) in unit of \( \text{cm}^3 \text{ s}^{-1} \) is derived from Equation 8.61, which yields

\[
k_3 = k_1/8 = 1.73 \times 10^{-5} T^{-1.025} e^{(-52000/T)}.
\] (8.64)

The corresponding chemical timescales of these four reactions are

\[
t_{\text{chem}}^1 = \frac{1}{n_H k_1} = \frac{0.72 \times 10^4}{n_H} T^{1.025} e^{52000/T}
\]

\[
t_{\text{chem}}^2 = \frac{1}{n_H^2 k_2} = \frac{0.69 \times 10^{26}}{n_H^2} T^{1.54}
\] (8.65)

\[
t_{\text{chem}}^3 = \frac{1}{n_H k_3} = \frac{0.58 \times 10^5}{n_H} T^{1.025} e^{52000/T}
\]

\[
t_{\text{chem}}^4 = \frac{1}{n_H^2 k_4} = \frac{0.56 \times 10^{27}}{n_H^2} T^{1.54}.
\]

in unit of \( s \). In general, the timescales are dependent on both density and temperature. The timescale of the collisional dissociation \( t_1 \) and \( t_3 \) are inversely proportional to the density, while the ones of the three-body recombination \( t_2 \) and \( t_4 \) are inversely proportional to density squared.

8.4.3.2 Glassgold and Huggins critical effective temperature

As presented in equations 8.50 and 8.51, at high densities close to the surface and in the absence of dust, the hydrogen molecule is formed with rate coefficients \( k_2 \) and \( k_4 \), while it is destructed with rate coefficients \( k_1 \) and \( k_3 \). Taking them into account, chemical equilibrium yields:

\[
1 = \frac{k_2 x^3 + k_4 x^2 x_2}{k_1 x_2 x + k_3 x_2^2} n_H
\]

\[
= \frac{k_2 (1 - 2x_2)^3 + k_4 x_2 (1 - 2x_2)^2}{k_1 x_2 (1 - 2x_2) + k_3 x_2^2} n_H.
\] (8.66)
We rewrite Equation 8.66 as:

\[
(1 - 2x_2^2)x_2 + \frac{k_2}{k_4}(1 - 2x_2^2)^3 - \frac{1}{n_H} \left[ \frac{k_1}{k_4}(1 - 2x_2)x_2 + \frac{k_3}{k_4x_2^2} \right] = 0. \quad (8.67)
\]

Solving Equation 8.67 allows us to determine \( x_2 \), the equilibrium fractional abundance of molecular hydrogen \( x_2 \). Since the reaction rate coefficients are a function of temperature, the hydrogen fractional abundance at the stellar photosphere is a function of both stellar temperature and density. Figure 8.5 shows the relation between \( \text{H}_2 \) fractional abundance and stellar temperature for several density values. Depending on the stellar temperature, hydrogen can be either in molecular or in atomic form at the stellar surface. The hydrogen is in molecular form for "cold" stars, and in atomic form for "hotter" stars. This transition point varies over the density of stellar surface. For stars with \( n_H \geq 10^{14} \text{ cm}^{-3} \), the transition is around at 2500 K, which means that stars with \( T_\star \leq 2500 \text{ K} \) contains mostly molecular hydrogen, and mostly atomic hydrogen with \( T_\star > 2500 \text{ K} \). That was concluded also by (Glassgold and Huggins, 1983). The use of the rates by Forrey (2013) leads to a shift of this critical temperature of about 200K towards lower temperatures. This corresponds to a 4-fold increase of atomic hydrogen in the molecular side of the diagram, which has a similar impact on the predicted HI emissivities for given hot (i.e., hotter than the critical temperature) AGB stars observations of HI.

### 8.4.4 Collisional dissociation of H\(_2\) level by level

Collisional dissociation of \( \text{H}_2 \) is included in the Paris-Durham code, as it is important for dissociative shocks. In the dilute conditions of the ISM, LTE is not realized for the \( \text{H}_2 \) levels, and it is important to consider the dissociation level by level (Le Bourlot et al., 2002). Our level by level implementation assumes that the dissociation energy barrier for a given level is lowered precisely by its excitation energy:

\[
D_i = D_{00} e^{T_i/T} \quad (8.68)
\]

where \( D_{00} \) is the rate for collisional dissociation of the ground level \( (v = 0, J = 0) \). In the former version of the Paris-Durham code, the input list of chemical reactions assumes that the rate for \( D_{00} \) is given. For instance, the rate used for \( \text{H} + \text{H}_2 \rightarrow 3\text{H} \) was \( D_{00} = 10^{-10} \exp(-52000/T) \text{ cm}^3 \text{s}^{-1} \) (Dove and Mandy, 1986). However, the rates we provide now are for the total rate at LTE:

\[
D_{\text{LTE}} = \sum_i D_i \frac{g_i}{Z(\text{H}_2)} e^{-T_i/T} = D_{00} \sum_i \frac{g_i}{Z(\text{H}_2)} \gg D_{00}. \quad (8.69)
\]
In order to recover the correct rate at LTE near the stellar surface, and to keep our assumed level by level behavior in the dilute ISM phase, we therefore need to use the new prescription:

\[ D_i = D_{LTE} \frac{Z(H_2)}{\sum_i g_i} e^{T_i/T} \]  \hspace{1cm} (8.70)

which we implemented in the Paris-Durham code. Note that in our assumption, the barrier compensation due to excitation exactly compensates the Boltzmann factor: at LTE, each level contributes roughly in proportion of its statistical weight. This means in particular that we need to include a large number of H$_2$ levels in order get convergence for the hydrogen chemistry (see Figure 8.6). It would be desirable to implement a more efficient treatment for the discarded levels in order to achieve better computational efficiency for the winds. For example, one could assume that all discarded levels are populated as a Boltzmann population with respect to the last included level.
8.5 Extinction

Radiation from nearby stars is able to photo-ionize species and photo-dissociate molecules. Dust grains, however, will absorb the radiation and protect the chemical elements against photo-destruction. In the Paris-Durham shock code, the impact of the dust is modeled through the extinction variable \( A_v \). This is computed with a plane-parallel geometry. We also assume the interstellar radiation comes from upstream (Lesaffre et al., 2013), allowing us to integrate \( A_v \) alongside the model calculation:

\[
A_v^{\text{shock}} = A_{v0} + \int_{z_0}^{z} dz \alpha_{A_v} n_H
\]  

(8.71)

where \( A_{v0} \) is the starting extinction upstream of the shock and \( \alpha_{A_v} = 5.34 \times 10^{-22} \text{cm}^2 \) is a cross-section parameter which characterizes the optical properties of interstellar dust and their abundance with respect to \( n_H \).

In the wind situation, however, the chemically active radiation comes from the outside, at the tip of the wind, and we don’t know the density profile. However, we can nevertheless resort to approximations, as many authors before (e.g., Mamon et al. 1987). We assume
that the terminal velocity is already reached and that the density profile decays exactly as $1/r^2$. We also assume that the dust properties behave like standard ISM dust

$$A_v^{\text{wind}}(r) = A_v^{\text{iso}} + r \alpha_{A_v} n_H(r).$$

(8.72)

As $n_H$ varies as $1/r^2$, this expression diverges close to the star, where the extinction is so large that the photo-reactions don’t matter anymore. Far from the star, dust properties are more likely to behave as standard ISM dust, so the approximation is also appropriate. We checked that this yields photo-dissociation profiles comparable to the results found by Mamon et al. (1987), as illustrated in Figure 8.7.

Self-shielding functions for the photo-dissociation of $H_2$ and CO was also included in the Paris-Durham code (Lee et al., 1996, Lesaffre et al., 2013). These functions require column-densities as entry parameters, and we made similar assumptions as for Equation 8.72:

$$N_{H_2}^{\text{shield}} = N_{H_20} + r n(H_2)$$

(8.73)

and

$$N_{CO}^{\text{shield}} = N_{CO} + r n(CO).$$

(8.74)
Extinction also occurs in the line cooling: when photons need to go through a large quantity of matter to find the exit to the circumstellar envelope, radiation becomes optically thick, and line cooling effectively shuts off. This is accounted for by a velocity-gradient parameter in the molecular cooling tables of Neufeld and Kaufman (1993). We use their recommended value for spherical symmetry:

\[
\frac{dv_n}{dz} = 27 \frac{c_s}{2} \frac{v_n}{r} + 2 \frac{v_n}{r}.
\]  

(8.75)

### 8.6 Validation

Finally, we ran a stellar wind model for GX Mon star and we checked that the dynamical properties of the gas that we calculated are comparable to the results of Justtanont et al. (1994), as showed in Figure 8.8
\textbf{Figure 8.8}: Dynamical properties of gas in the CSE of GX Mon star (bottom) for comparison with Justtanont et al. (1994)'s model (top). The blue line in the bottom panel is the speed of sound. GX Mon parameters: $M_*=M_\odot$, $\dot{M}_*=7.2\times10^{-6}\,M_\odot\,\text{yr}^{-1}$, $T_*=2500\,\text{K}$. 

Chapter 9

MODELS

9.1 IRC +10216 star

9.1.1 Hydrodynamics

IRC +10216 or CW Leonis is the nearest carbon-rich AGB star, at a distance of \( \sim 130 \) pc, and it has been extensively observed. IRC +10216 is believed to be close to the stage where it becomes a protoplanetary nebula (e.g., Skinner et al. 1998). Because of this, there is no doubt that IRC-10216 has high mass-loss rate (\( \approx 2 \times 10^{-5} \) \( M_\odot \) yr\(^{-1} \); i.e., Crosas and Menten 1997; Groenewegen et al. 1998). The main parameters of IRC +10216 are summarized in Table 9.1.

The effective temperature is uncertain due to the thickness of the dust envelope. Quoted values are 2300 K (Cohen, 1979), 2330 K (Ridgway and Keady, 1988), 2200 K (Ivezić and Elitzur, 1996), or 1915 – 2105 K (Bergeat et al., 2001). We, therefore, choose a mean value of 2200 K (Matthews et al., 2015).

The stellar mass is adopted to be 0.8 \( M_\odot \) as a mean value ranges from 0.7 to 0.9 \( M_\odot \) (Ladjal et al., 2010). Thanks to VLA observations, Menten et al. (2012) determines the luminosity of IRC +10216 at about 8640 \( L_\odot \). Adopting these stellar effective temperature and luminosity allows us to derive its radius \( R_\star \approx 4.5 \times 10^{13} \) cm. The carbon-to-oxygen ratio is assumed to be 1.5 (e.g., Willacy and Cherchneff 1998, Cherchneff 2006). Since we are concerned with dust condensation, and since IRC +10216 is an extreme carbon-rich star, we use the spherical amorphous carbon dust grains, with the refraction index from Maron (1990) (see subsection 8.3.2).
### Table 9.1: Input model parameters for IRC +10216.

| Parameter                        | Value               |
|----------------------------------|---------------------|
| Stellar radius ($R_*$)           | $4.5 \times 10^{15}$ cm |
| Stellar effective temperature ($T_*$) | 2200 K             |
| Stellar luminosity ($L_*$)       | $8640 L_\odot$      |
| Stellar mass ($M_*$)             | $0.8 M_\odot$       |
| Mass-loss rate ($\dot{M}_*$)     | $2 \times 10^{-5} M_\odot$ yr$^{-1}$ |
| Carbon/oxygen ratio ($C/O$)      | 1.5                 |
| $\Gamma$                        | $\simeq 1.25$       |

#### 9.1.1.1 Freely expanding wind region

Using the parameters of Table 9.1, the physical profiles of the gas in the freely expanding wind region are shown in Figure 9.1. The *top panel* indicates that the terminal velocity is about 14 km s$^{-1}$, which is in good agreement with the observed value for IRC +10216 (e.g., Olofsson et al. 1993, Knapp et al. 1998). In addition, the gas flow starts reaching this stationary value at $\sim 10^{15}$ cm, which is also in good agreement with Agündez et al. (2012).

Inside the dust-free region, we fit the gas kinetic temperature and the gas number density to a power-law of radius as $r^\alpha$. The number density varies with $\alpha = -2$. While the gas temperature varies with $\alpha = -0.33$, where $r \leq 6.5 \times 10^{13}$ cm.

#### 9.1.1.2 Detached shell region

Matthews et al. (2015) reported the discovery of a faint HI shell at a radius $\sim 1.2 \times 10^{18}$ cm around the IRC +10216 star. The kinematics of this shell are consistent with matter that has been slowed down by interaction with the ISM. In addition, the HI emission from the freely expanding wind is broad (Hoai et al., 2015), therefore it is not the main reason for this detection. Based on the FUV radial intensities obtained by GALEX observations (see subsection 1.3.2), Sahai and Chronopoulos (2010) estimated the detached shell defined by a termination shock with the inner radius of $\sim 8.58 \times 10^{17}$ cm and the outer radius of $\sim 1.008 \times 10^{18}$ cm.

Since we neglect the effect of the magnetic field, we run a 1D J-type shock (see subsubsection 4.1.3.2) with entrance conditions provided in Table 9.2. The gas profiles in the termination shock region, plotted in the shock frame, are shown in Figure 9.2: the gas is decelerated by a factor of $\sim 4$ when it crosses the termination shock and is heated as mentioned in Hoai et al. (2015). It cools down thereafter, and its velocity continues to decrease via expansion, while the density is increasing. Due to the J-type shock character, the maximum of the gas temperature is large $\sim 10^4$ K, corresponding to the 14 km s$^{-1}$
Figure 9.1: Physical profiles of gas in the freely expanding wind region of the IRC+10216’s CSE.

| Parameter      | Value   | Note                                           |
|----------------|---------|------------------------------------------------|
| \( n_H \)      | 52 cm\(^{-3}\) | Pre-shock density of H nuclei                   |
| \( A_\nu \)    | 0.022   | Extinction shield                               |
| \( N_0(H_2) \) | \(10^{20}\) cm\(^{-2}\) | Buffer H\(_2\) column density                   |
| \( N_0(CO) \)  | 0 cm\(^{-2}\)  | Buffer CO column density                        |
| \( G_0 \)      | 1       | External radiation field                        |
| \( \zeta \)    | \(3.10^{-17}\) s\(^{-1}\) | Cosmic ray flux                                 |
| \( OPR \)      | 3       | Pre-shock H\(_2\) ortho/para ratio             |
| \( v_s \)      | 14 km s\(^{-1}\) | Effective shock velocity                        |
| \( T \)        | 56 K    | Initial gas temperature                         |
| \( T_d \)      | 11 K    | Initial grain temperature                       |
| \( b_{||} \)    | 0       | No magnetic field                               |

Table 9.2: Main input parameters of termination shock in the CSE of IRC +10216. Note that we neglect the motion of the termination shock.
shock (see Lesaffre et al. 2013, equation 10). To sum up, Figure 9.3 displays the properties of gas in the CSE of IRC+10216, starting from the stellar surface through the CSE medium until its interaction with the ISM.

9.1.2 Hydrogen profile

The profile of hydrogen in the CSE of IRC +10216 is displayed in Figure 9.4. At such a low effective temperature (2200 K), the IRC+10216 star should have a surrounding CSE mostly composed of molecular hydrogen. Figure 9.3 indicates that the initial gas density \( n_{H} \) in the stellar photosphere is \( \sim 10^{14} \text{ cm}^{-3} \). Reporting this value in Figure 8.5, we see that the initial fractional abundance of atomic hydrogen in the stellar photosphere is \( \sim 0.1 \), while that of molecular hydrogen is \( \sim 0.45 \).

Close to the star, where the wind starts to launch, the velocity of the gas is increasing but its absolute value is still small, so that the dynamical timescale remains longer than the chemical timescale. Thus the chemistry including the three-body reactions impacts on the variation of the hydrogen abundances. The chemical timescale depends on both the density and the temperature of the gas. However, these timescales weakly depend on the density since its decreasing slope is less steep than the temperature (Figure 9.1). Therefore, the timescales of the three-body recombination \( t_{2}^{\text{chem}} \) and \( t_{4}^{\text{chem}} \) are shorter than the
ones of the collisional dissociation $t_1^{chem}$ and $t_3^{chem}$ (subsection 8.4.3). This characterizes the cumulation of the molecular hydrogen in the subsonic region. In addition to this, when forming dust grains, the hydrogen abundance is enhanced furthermore due to its formation on grain surface by adsorbing atomic hydrogen. The hydrogen abundance therefore is significantly increased ($x(H_2) \sim 0.495$, corresponding to $x(H) \sim 0.01$).

At such a higher radius, where the gas velocity is high enough, the dynamical timescales becomes shorter than the chemical timescales. Hence the chemical reactions could not occur, which makes the abundance of hydrogen freeze-out.

At the radius of $\sim 9 \times 10^{17}$ cm, where the detached shell appears, the chemical timescale turns back to be shorter than the dynamical timescale because the termination shock slows down the gas. The abundance of molecular hydrogen is now reduced due to the photo-dissociation by the ISRF. Crossing this region, the abundance of H terminates at $\sim 0.2$, with a corresponding abundance of atomic hydrogen at $x(H_2) \sim 0.4$. 
9.2 Y Canum Venaticorum (Y CVn)

9.2.1 Hydrodynamics

Y CVn is a spectral-type J carbon-rich star. Contrary to IRC +10216, the evolution state of Y CVn is not well known. Some authors have suggested that it could evolve on the red giant branch (RGB), in which the carbon composition might be produced by the core He flash (Dominy, 1984). However, the high mass-loss rate, as derived from observations of the detached dust shell (Izumiura et al., 1996) confronts the belief that Y CVn is on the AGB phase. Other authors suggest that it has not reached the thermal pulse yet, because there is no detection of technetium (Little et al., 1987) and a lack of s-process elements (Utsumi, 1985), which are enhanced by the Third Dredge-up process. This convection process is an indication of the TP-AGB phase (see subsection 1.3.2). Its luminosity ($L \sim 6200 \, L_\odot$) (Libert et al. 2007), which is converted from a bolometric magnitude of 1.96 (Le Bertre et al. 2001) at a distance of 218 pc (Perryman et al. 1997), probably locates Y CVn on the early AGB.

Nevertheless, the distance to Y CVn is also uncertain. According to the analysis of Perryman et al. (1997) on the Hipparcos parallax measurement, the distance is estimated at about 218 pc, while other authors come up with different results by re-analyzing this measurement. For instance, the distance is approximated as $\sim 272 \, \text{pc}$ (Knapp et al. 2003) or $\sim 312$ (van Leeuwen 2007). In this work, we take the value of $\sim 218 \, \text{pc}$ as Libert et al. (2007).
### Table 9.3: Input model parameters for Y CVn.

| Parameters                             | value         |
|----------------------------------------|---------------|
| Stellar radius ($R_*$)                 | $2.45 \times 10^{13}$ cm |
| Stellar effective temperature ($T_*$)  | 2760 K        |
| Stellar luminosity ($L_*$)             | 6200 $L_\odot$ |
| Stellar mass ($M_*$)                   | 1.6 $M_\odot$ |
| Mass-loss rate ($\dot{M}_*$)           | $1.5 \times 10^{-7}$ $M_\odot$ yr$^{-1}$ |
| Carbon/Oxygen ratio ($C/O$)            | 1            |
| $\Gamma$                               | $\approx 1.015$ |

The effective temperature of Y CVn is $\sim 2760$ K (Bergeat et al. 2001). The mass-loss rate is adopted as $1.5 \times 10^{-7}$ $M_\odot$ yr$^{-1}$ (Schöier et al. 2002). Unfortunately there is no clear constraint on its mass, we thus use the arbitrary value of 1.6 $M_\odot$ (mass of RS CnC star) following a suggestion by Thibaut Le Bertre. The main parameters of Y CVn are listed in Table 9.3.

#### 9.2.1.1 Freely expanding wind region

The implementation of the stellar wind model with these parameters gives us the physical properties of the gas in the region of free expansion. The top panel of Figure 9.5 indicates that a terminal wind velocity of about 8.7 km s$^{-1}$, which is similar to the value obtained from the estimate standard radiative modeling of CO observations (Olofsson et al. 1993, Schöier and Olofsson 2001), or from high-resolution observations of the CO spectrum (Knapp et al. 1998). We also fit the thermal properties of the gas to a power law in radius as $r^\alpha$. $\alpha$ equal $-1.32$ in the range $3.22 \times 10^{13}$ cm $\leq r \leq 3.1 \times 10^{15}$ cm. Beyond this range, it turns positive due to the photoelectric heating effect. $\alpha = -1.92$ where $3.1 \times 10^{15}$ cm $< r \leq 1.5 \times 10^{16}$ cm, and $\alpha = -0.18$ where $r > 1.5 \times 10^{16}$ cm.

#### 9.2.1.2 Detached shell region

A shell in the HI 21-cm line in Y CVn was detected by Le Bertre and Gérard (2004), Gérard and Le Bertre (2006) and Libert et al. (2007) with the Nançay Radio Telescope (NRT), and Matthews et al. (2013) with the VLA telescope. As discussed in subsubsection 9.1.1.2, a detached shell is likely to be the main cause for this emission. Thanks to the ISO 90 $\mu$m observation, Izumiura et al. (1996) clearly showed a quasi-circular shell with an inner radius of $r_{in} \approx 5.48 \times 10^{17}$ cm and an outer radius of $r_{out} \approx 7.24 \times 10^{17}$ cm - $\approx 9.98 \times 10^{17}$ cm by adopting the distance of $\sim 218$ pc. Therefore, we turn on the J-shock, whose input parameters are in Table 9.4, at a radius of $r_{in}$.

Figure 9.6 shows the gas profiles in the termination shock of Y CVn in shock frame, Like in subsubsection 9.1.1.2, this figure indicates a factor of 4 of the acceleration of gas when...
Figure 9.5: Physical profiles of gas properties in the freely expanding wind region of the Y CVn CSE.

| Parameter   | Value      | Note                              |
|-------------|------------|-----------------------------------|
| $n_H$       | 2.06 cm$^{-3}$ | Pre-shock density of H nuclei |
| $A_v$       | 0.0004     | Extinction shield                 |
| $N_0(H_2)$  | $10^{20}$ cm$^{-2}$ | Buffer H$_2$ column density |
| $N_0(CO)$   | 0 cm$^{-2}$ | Buffer CO column density         |
| $G_0$       | 1          | External radiation field          |
| $\zeta$     | 3.10$^{-17}$ s$^{-1}$ | Cosmic ray flux     |
| $OPR$       | 3          | Pre-shock H$_2$ ortho/para ratio  |
| $v_s$       | 8.7 km s$^{-1}$ | Effective shock velocity         |
| $T$         | 73 K       | Initial gas temperature          |
| $T_d$       | 12.8 K     | Initial grain temperature        |
| $b_{\parallel}$ | 0      | No magnetic field                |

Table 9.4: Main input parameters of termination shock in the CSE of Y CVn. Note that we neglect the motion of the termination shock.
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FIGURE 9.6: Physical profiles of the gas in the detached shell region of the Y CVn CSE.

FIGURE 9.7: Physical profiles of the gas in the CSE of Y CVn.
it crosses the termination shock and is heated. The gas flow also cools down thereafter, and its velocity also continues decreasing via expansion, while the density is increasing. Due to the J-type shock character, the maximum of the gas temperature is also large $\sim 2500$ K. To sum up, Figure 9.7 displays the properties of gas in the CSE of YCVn, starting from the stellar surface through the CSE medium until its interaction with the ISM.

9.2.2 Hydrogen profile

The profile of molecular and atomic hydrogen is displayed in Figure 9.8. Because of its high effective temperature ($2760$ K), the CSE around YCVn is expected to contain mostly atomic hydrogen (HI). Similar to subsection 9.1.2, the variation of hydrogen in the CSE of YCVn is explained by the interplay between dynamical and chemical timescales. On the stellar photosphere, the initial fractional abundance of atomic hydrogen $\sim 0.94$, and that of molecular hydrogen is $\sim 0.03$ due to the gas density $n_H \sim 10^{13}$ cm$^{-3}$ (Figure 9.7). In the innermost region, molecular hydrogen is enhanced through the three-body recombination reactions. Both profiles freeze-out when the gas velocity is sufficient high and atomic hydrogen is finally more enhanced due to the photo-dissociation of molecular hydrogen by the termination shock and the ISRF.
9.3 HI modeling

As discussed in section 3.3, the 21-cm line ($\lambda = 21$ cm) of HI is an excellent probe of the CSE of AGB stars. The radiation comes from the transition between the two split levels of atomic hydrogen in its ground state, which is caused by the interaction between the electron spin and the nuclear spin. This splitting is known as hyperfine structure (Figure 9.9). The relevant frequency of the 21-cm line radiation is:

$$\nu_{10} = \frac{c_1}{\lambda} = 1.420 \times 10^9 \text{ s}^{-1}. \quad (9.1)$$

The probability of this transition is defined by:

$$A_{10} = \frac{64\pi^4}{3\hbar c_1^3} \left| \frac{e\hbar}{2m_e c_1} \right|^2 = 2.8688 \times 10^{-15} \text{ s}^{-1} \quad (9.2)$$

where $\hbar = h/2\pi$ is the reduced Planck’s constant, $e$ is the charge of the electron, and $m_e$ is its mass. This extremely small value means that, for a single atomic hydrogen, the emission of radiation in the 21-cm line pasts $\sim 10^7$ yr, therefore it is very difficult to observe. As the total number density of atomic hydrogen is very large in the ISM, this radiation, however, is easy to detect by radio telescopes.

The specific intensity of the radiation $I_\nu$ changes according to the absorption and/or emission processes along the ray (Figure 9.10). The radiative transfer equation states that

$$\frac{dI_\nu}{ds} = \epsilon_\nu - k_\nu I_\nu \quad (9.3)$$
where $\epsilon_\nu$ and $k_\nu$ are the emissivity and absorption coefficients in the line of sight $ds$. The analytical solution of Equation 9.3 is

$$I_\nu = e^{-\int_0^s k_\nu ds} \left( \int_0^s \epsilon_\nu e^{\int_0^s k_\nu ds'} ds + \text{const.} \right)$$  \hspace{1cm} (9.4)

As in subsubsection 8.2.1.2, we consider the two levels system, named 0 (lower) and 1 (upper) of the 21-cm line (Figure 9.9). Three processes are considered to formulate $\epsilon_\nu$ and $k_\nu$: (1) spontaneous emission from the upper to the lower level, (2) absorption from the lower to the upper level, and (3) stimulated emission from the upper to the lower level.

Differential energy emitted spontaneously:

$$dE_e(\nu) = h\nu n_1 A_1 c_1 \phi(\nu) d\nu \frac{d\omega}{4\pi} dt dV.$$  \hspace{1cm} (9.5)

Differential energy absorbed:

$$dE_a(\nu) = h\nu n_0 B_0 \frac{4\pi}{c_1} I_\nu \phi(\nu) \frac{d\omega}{4\pi} d\nu dtdV.$$  \hspace{1cm} (9.6)

Differential energy of stimulated emission:

$$dE_s(\nu) = h\nu n_1 B_1 \frac{4\pi}{c_1} I_\nu \phi(\nu) \frac{d\omega}{4\pi} d\nu dtdV.$$  \hspace{1cm} (9.7)

where $n_1$ and $n_0$ are the densities of the upper level, and the lower level, respectively. $dV = d\sigma ds$ is the unit volume. $A$ and $B$ are the Einstein coefficients, which were introduced in subsubsection 8.2.1.2. As in section 5.6, we also introduce a line broadening function $\phi(\nu)$ due to the thermal Doppler effect.
Chapter 9. Models

The intensity of the radiation is the contribution the three terms above, which yields:

\[ dI_\nu d\omega d\nu dt d\sigma = dE_e(\nu) + dE_a(\nu) - dE_s(\nu) \]

or

\[ \frac{dI_\nu}{ds} = \frac{\hbar \nu_0}{4\pi} A_{10} n_1 \phi(\nu) + \frac{\hbar \nu_0}{c_l} I_\nu \phi(\nu)[n_1 B_{10} - n_0 B_{01}] \]

By comparing Equation 9.8 to Equation 9.3, the emission and adsorption coefficients are:

\[ \epsilon_\nu = \frac{\hbar \nu_0}{4\pi} A_{10} n_1 \phi(\nu) \] (9.9)

and

\[ k_\nu = \frac{\hbar \nu_0}{c_l} \phi(\nu)(n_0 B_{01} - n_1 B_{10}) \]. (9.10)

Using the relation of the Einstein coefficients (Equation 8.25 and Equation 8.26) and assuming the system is in LTE (Equation 8.31), we have:

\[ k_\nu = \frac{c_l^2}{8\pi \nu_{10}^2} \phi(\nu) n_0 \frac{g_1}{g_0} A_{10} \left(1 - e^{-\frac{\hbar \nu_{10}}{k_B T}}\right) \] (9.11)

At small frequency (\(\hbar \nu_{10}/k_B \sim 0.07 \text{ K}\)), one can replace \( e^{-\hbar \nu_{10}/k_B T} \) by 1 − \( \hbar \nu_{10}/k_B T \) and Equation 9.11 can be rewritten as:

\[ k_\nu = \frac{c_l^2}{8\pi \nu_{10}^2} \phi(\nu) n_0 \frac{g_1}{g_0} A_{10} \frac{\hbar \nu_{10}}{k_B T} \] (9.12)

For 21-cm line, \( g_0 = 1 \) and \( g_1 = 3 \), and the population is in statistical equilibrium \( n_0 = 1/4n_H \) and \( n_1 = 3/4n_H \), where \( n_H \) is the total density of hydrogen in ground state. In practice, observers mostly express the spectra as a function of the radial velocity \( v_r \). Hence, we replace \( \phi(\nu) \sim \phi(v_r) \). The line function as a function of \( v_r \) is defined by:

\[ \phi(v_r) = \frac{\lambda}{\sqrt{2\pi} \sigma} e^{-\frac{(v_{rad} - v_r)^2}{2\sigma^2}} \] (9.13)

where \( \sigma^2 = (k_B/m_H)T \) is the thermal velocity of atomic hydrogen. The emission velocity \( v_{rad} \) is illustrated in Figure E.1. With these transformations, the emission coefficient (Equation 9.9) and the adsorption coefficient (Equation 9.12) can be rewritten as:

\[ \epsilon_{v_r} = \frac{3\hbar \nu_{10}}{16\pi} n_H A_{10} \phi(v_r) \] (9.14)

\[ k_{v_r} = \frac{3c_l^2}{32\pi \nu_{10}^2} n_H A_{10} \frac{\hbar}{k_B T} \phi(v_r) \] (9.15)
and the specific intensity \( (\text{Equation 9.4}) \) is become:

\[
I_r(r_0) = e^{-\int_{-s_{\text{out}}}^{s_{\text{out}}} k_{vr} ds} \left( \int_{-s_{\text{out}}}^{s_{\text{out}}} \epsilon_{vr} e^{\int_{-s_{\text{out}}}^{s_{\text{out}}} k_{vr} ds'} ds' + \text{const} \right). \tag{9.16}
\]

As discussed earlier, we consider a spherical geometry for the CSE around an AGB star. In that simple case, the computational technique of these integrations in \( \text{Equation 9.16} \) is described in Appendix E. The only needed parameter is \( R_{\text{out}} \), which defines the outer radius of the detached shell. Finally, the observed flux density on earth is defined by:

\[
F_{vr} = \frac{\int_0^{R_{\text{max}}} 2\pi r_0 I_r(r_0) dr_0}{d^2}. \tag{9.17}
\]

where \( d \) is the distance of the star and \( R_{\text{max}} \) is the size of the observation beam. We also verify our method by using the same physical properties as Hoai et al. (2015) and comparing the calculated flux density with their method. Figure E.2 is flux density calculated for the two cases of \( \dot{M}_* = 10^{-7} \, M_\odot \, \text{yr}^{-1} \) and \( \dot{M}_* = 10^{-5} \, M_\odot \, \text{yr}^{-1} \), which are compatible to Hoai et al. (2015)’s figure(2).

### 9.3.1 HI modeling for IRC +10216

Figure 9.11 shows the line profile of the HI 21-cm line profile in the CSE of IRC +10216 with \( \times 100” \) beam side of radius (corresponding to \( R_{\text{max}} \sim 9.45 \times 10^{16} \, \text{cm} \)). To our knowledge, it is the first modeling attempt. \textit{Top panel} shows the flux density profile, which is computed by using the physical profile of IRC +10216 (Figure 9.3) extended up to \( R_{\text{out}} \sim 1.008 \times 10^{18} \, \text{cm} \) (subsubsection 9.1.1.2). The emission from the detached shell characterizes the central peak, while \textit{double-horned} structure identifies the freely expanding wind. \textit{Bottom panel} shows the zoom-in profile in comparison with the Green Bank Telescope (GBT) observations (Matthews et al., 2015). The observational data is the difference between the spectrum integrated over a 100” aperture on the IRC +10216 position with reference spectra extracted over 1100” east of the star (outside the HI shell). Unfortunately, there are two drawbacks in our model: first, the simulated flux density is about 10 times higher than the value inferred from observations in the freely expanding region, which means that the abundance of atomic hydrogen computed by our model is about 10 times higher than it should be in this regions. Second, our model greatly overestimates the emission of the detached shell.

Now, if we consider the motion of the termination shock (see Appendix D for detail) and assume that the density of the ISM is on the order of the stellar wind medium, the termination shock’s frame will move at the velocity \( u_s = v_w/2 \). Therefore, the input shock velocity now is \( v_w/2 = 7 \, \text{km} \, \text{s}^{-1} \) in the termination shock’s frame. Furthermore, instead of using the J-type, we also consider a C-type shock for the magnetized ambient medium with the typical value \( b = 1 \). Updating the parameters in Table 9.2 on these new
values, we recompute the termination shock. Because of the lower compression factor, the emission in the detached shell with a C-type shock is now negligible and we can free ourselves from the second problem above (Figure 9.12).
Figure 9.11: *(Top)* HI 21-cm line profile in the CSE of IRC +10216 obtained by model with 14 km s$^{-1}$ J-type termination shock. *(Bottom)* Comparison with GBT observations.
Figure 9.12: Same as Figure 9.11, but using 7 km s\(^{-1}\) C-type terminal shock.

### 9.3.2 HI modeling for Y CVn

Figure 9.13 shows the HI 21-cm line profile in the CSE of Y CVn computed by our model with only one free parameter \(R_{\text{max}}\) \((R_{\text{out}} = R_{\text{max}})\). Top panel shows the comparison with NRT observations (Libert et al., 2007) and with the fit from a parametric model with 5 free parameters (Hoai et al., 2015). Bottom panel shows the comparison with the *Five hundred-meter Aperture Spherical radio Telescope* (FAST) simulation (Hoai et al., 2017), which is based on VLA observations (Matthews et al., 2013).

Our model matches quite well the observations, however, the width of the central line is narrower than observations, which means that the temperature computed by our model is cooler than the observational one in the detached shell. On contrary, the width of the wings is broader, which is synonymous with the fact that the temperature computed by our model is hotter than the observational one in the freely expanding wind region. Therefore, our total flux integrated over velocity is quite comparable to observations. It is about 2.14 Jy km s\(^{-1}\) from our model and about 2.34 Jy km s\(^{-1}\) from NRT observations.
Figure 9.13: Y CVn HI 21-cm line profile computed by the HI model in comparison with the NRT observations (top panel) and the FAST simulation (bottom panel). The profile obtained with $R_{\text{max}} \sim 7.47 \times 10^{17}$ cm.
Chapter 10

CONCLUSIONS AND PERSPECTIVES

10.1 Conclusions and remarks

In the last part of this thesis, we incorporated to the Paris-Durham shock code a few new physical ingredients to allow it to compute steady-state solutions of AGB winds. We included the geometrical dilution due to the spherical symmetry. We provided the code with the gravitation and radiation pressure forces, with the net effect of pushing the grains outwards and launching the wind. We modified the dynamical integration to help go through the sonic point. We now compute the dust temperature subject to radiation equilibrium. We modified the computation of the extinction so that the irradiation field is external and spherical geometry is accounted in the line cooling opacity. We found an approximation to easily account for gas heating by the radiation pumping near the stellar surface. Finally, we added three-body reactions necessary to form H$_2$ at the high densities experienced near the stellar surface.

With this new powerful tool, we started to examine the time-dependent conversion of atomic to molecular hydrogen along the wind trajectories, and we proceeded to model two AGB stars with surface temperatures below and above the critical temperature for hydrogen to be in atomic or molecular form. In the "low" temperature case, we show that hydrogen quickly becomes molecular in the wind, which might explain the difficulty to detect HI with instruments such as the VLA in AGB winds.

We have tried to reproduce the HI 21-cm line profile from the CSE of the AGB stars in two example cases: IRC +10216 and Y CVn. In the case of IRC +10216, our model can produce the "double-horned" structure but it contains about 10 higher of the atomic
hydrogen than the observational expectation. In the case of Y CVn, our model reproduces quite well observations but the temperature computed from our model seems cooler than observations in the detached shell region. Hopefully, the FAST telescope will provide us with better sensitivity in the future and thus bring better statistics for a greater number of stars.

10.2 Perspectives

Although $H_2$ is the dominant molecular species in the ISM, $H_2$ is a tracer only at the high temperatures caused by shocks and at large scales when excited by UV radiation from the ISM. Alternatively, CO is one of the major molecules used to determine the dynamics of stellar wind and also its interaction with the ISM. Therefore, we aim at updating the chemical network for CO and calculating CO emission from stellar winds. The CO chemistry will have to incorporate more three-body reactions which are not yet present in the Paris-Durham code. Fortunately, now that the framework has been developed in the code, it will be simply a matter of updating the network input file, and finding which reactions are relevant. Once we have a good description of the CO chemistry, we will be in a good position to synthesize the results of many observable data (e.g., Truong-Bach et al. 1991, Groenewegen et al. 1998, Knapp et al. 1998, Hoai et al. 2014) thanks to the post-processing tools for the emissivity of CO lines (and other molecules) developed by Gusdorf et al. (2008) which can be directly fed to outputs of the Paris-Durham code (assuming spherical symmetry). In particular, we shall be able to control the validity of the LTE approximation made to infer temperatures from observations by Hoai et al. (2014) and Nhung et al. (2015a).

In these stellar wind models, the formation and evolution of circumstellar dust grains is not yet properly treated. We assumed that the grain radii follow a “standard” (MRN) grain-size distribution as soon as the gas temperature is lower than the condensation temperature. The slope of -3.5 (MRN distribution) is believed to be appropriate for typical interstellar dust (Mathis et al., 1977), while other studies suggest that it should be steeper for circumstellar dust shells (Dominik et al., 1989). Therefore, we will thus aim at studying in a consistent way the processes of coagulation of the circumstellar dust grains. One place to start would be to introduce Hirashita’s simple coagulation model in the code, with a bin size by bin size treatment (Hirashita and Omukai, 2009).

Pulsations are the dominant theory to lift the wind from the stellar surface. Material is pushed away from the star during each period of pulsation, then the gravitational force becomes dominant and forces them backward on to the star. The falling flow meets the upward drafts from the next pulsation, and are slowed down by shocks and pushed outward
Figure 10.1: Positions of selected mass shells in AGB atmospheres showing how pulsation can affect on the large scale motion of the gas (Hoefner and Dohrmann, 1997).

The process is repeated until the gas flow condensates solids and gets accelerated by the newly formed dust grains (see Figure 10.1). With a prescribed scaling for the shock strength vs. radius, we can trigger a shock in the flowing wind every period thanks to the versatility of the Paris-Durham shock code. This way, we could model such thermally pulsing winds with our shock code.

Thanks to ALMA high resolution data, Decin et al. (2015) found evidence for a spiral structure in inner wind of IRC +10216, which could be caused by a binary companion. We thus started to simulate the trajectory of a wind in a binary star system in the hypersonic regime. In the hypersonic regime, the pressure gradients are negligible, and the fluid parcel's paths can be computed independently from each other. This allows to recover spiral shocks structures where two flows meet as shown in Figure 10.2. We are currently able to model only trajectories in the equatorial plane, and the full 3D structure of the wind still escapes us, but we feel this can eventually be done, and we could generate in 3D each individual fluid parcel trajectory, as well as the characteristic of the 2D manifold of the shocks generated by inter-penetrating trajectories. We then plan to post-process
with our code the thermal and chemical properties of the gas along these trajectories to reproduce detailed observations and help interpret ALMA data.

The above remark on hypersonic flows is valid for more simple winds and we expect to recover wind asymmetries such as detected by Hoai et al. (2016) on W Aquilae star. This simple assumption can also be used to model the influence of a magnetic field, provided we neglect the back-reaction of the flow of the field (i.e., we can easily compute fluid parcel trajectories for a prescribed magnetic field configuration).

We thus claim that such simple models can easily provide predictions for complex dynamics and chemistry, and greatly help observers interpret the ever increasing wealth of details unveiled by the new generations of instruments such as ALMA. Thanks to their policy of quick release, ALMA observations are a gold mine for researchers who have not yet easy access to powerful facilities, as is still the case in Vietnam. We hope this work will help foster research projects in Vietnam’s flowering astrophysics for quite a few years to come.
Appendix A

H₂ Ortho/Para ratio

A molecule of hydrogen consists of two atoms. Each nucleus of these atoms can have its own spin. Depending on the direction of the nuclei’s spin, hydrogen can exist in two different configurations: ortho in which spins of both nuclei are in the same direction, and para in which spins of both nuclei are in the opposite direction. The difference between these two configurations manifests itself in the rotational energy of H₂. The rotational energy relates to the rotational quantum level \( J \) as \( E_J = B(J + 1) \), where \( B \sim 60.85 \) cm\(^{-1} \) is the rotational constant of H₂. In fact, the rotational ground state \( (J = 0) \) of hydrogen is only occupied by para \( (J = 0) \), while the lowest state \( (J = 1) \) for ortho \( (E_{rot} = 2B/k_B = 170.5 \text{ K}) \) is the first rotational state. The difference in rotational energy between ortho and para is thus \( \Delta E_J \sim 170 \text{ K} \).

At LTE, the ratio between ortho and para populations is:

\[
\frac{\text{ortho}}{\text{para}}(T_{rot}, \text{LTE}) = \frac{\sum_{J \text{ odd}} 3(2J + 1)e^{-E_J/k_BT_{rot}}}{\sum_{J \text{ even}} (2J + 1)e^{-E_J/k_BT_{rot}}}
\]  

(A.1)

The conversion between ortho-H₂ to para-H₂ can occur via four main mechanisms:

- First, proton from H₂ exchanges to H⁺, H₃⁺ or other cations: The proton exchange can be expressed as (Dalgarno et al., 1973)

\[
\text{H}_2(J=1) + \text{H}^+ \iff \text{H}_2(J=0) + \text{H}^+ + 170.5 \text{ K}
\]

(A.2)

This process is dominant at low temperature \( (T \leq 50 \text{ K}) \) (Flower et al., 2006) and releases the amount of energy 170 K. Therefore, if the temperature is less than 170 K, this reaction destroys ortho-H₂ and forms para-H₂.
• Second, active H and H$_2$ collisions (Dalgarno et al., 1973)

$$\text{H}_2(\text{para}) + \text{H} \rightleftharpoons \text{H}_2(\text{ortho}) + \text{H}. \quad (A.3)$$

This process mainly occurs at high temperature ($T \sim 3900$ K) and this is therefore negligible in cold molecular clouds.

• Third, interaction H$_2$ with interstellar dust grains:

$$\text{H}_2(\text{para}) + g \rightleftharpoons \text{H}_2(\text{ortho}) + g \quad (A.4)$$

This process is inefficient in low-velocity shocks (Timmermann, 1998).

• Fourth, the formation of H$_2$ onto the surface of dust grains:

$$\text{H(adsorb)} + \text{H(g)} \longrightarrow \text{H}_2 \quad (A.5)$$

This formation is not an important process in low-velocity shocks, because these shocks insufficiently produce atomic hydrogen and the rate coefficient for H$_2$ formation on dust is small (Timmermann, 1998).
Appendix B

Analytical expression of the distribution function of shock velocities for a parabolic bow shock

In section 5.2, we show the numerical methodology to calculate the distribution function of single shocks (defined by their velocities $u_\perp$) for a given arbitrary axisymmetric bow shock shape. Here we examine the accuracy of this method in the special case of the parabolic shape $z = x^2/R_0 - R_0$, where $R_0$ is a curvature radius. In this case, the norm of a segment $dl$ defined in Equation 5.1 becomes

$$dl = \sqrt{dx^2 + dz^2} = \sqrt{1 + \frac{4}{R_0^2} x^2} \, dx. \quad (B.1)$$

Therefore, the element area $ds$ (Equation 5.2) can be rewritten as:

$$ds = 2\pi \sqrt{1 + \frac{4}{R_0^2} x^2} \, x \, dx. \quad (B.2)$$

Following Equation 5.3, the tangent of the angle $\alpha$ is $\tan \alpha = dx/dz = 2R/x$, and noting that $\alpha = 90 - \theta$, $u_\perp = u_0 \cos \theta$, we can find the relation between $ds$ and $u_\perp$ as

$$ds = \frac{\pi}{2} \frac{R_0^2}{\sin^4 \alpha} \cos \alpha \, d\alpha = \frac{\pi}{2} \frac{R_0^2}{\cos^4 \theta} \sin \theta \, d\theta = \frac{\pi}{2} \frac{R_0^2}{u_0^3} \frac{du_\perp}{u_\perp^3}. \quad (B.3)$$
Integrating Equation B.3 over \( u_\perp \) from \( c \) to \( u_0 \), we obtain

\[
S_{\text{shock}} = \frac{\pi R_0^2}{2} u_0^3 \int_c^{u_0} \frac{du_\perp}{u_\perp^4} = \frac{\pi R_0^2}{6} \frac{u_0^3 - c^3}{c^3}.
\] (B.4)

Therefore, the probability density function in the case of a parabolic shape will be:

\[
PDF_{\text{parabola}} = \frac{ds}{\int ds} = \frac{3}{u_0^4(u_0^3 - c^3)}.
\] (B.5)

Figure B.1 shows the comparison in PDF calculation between our numerical method for arbitrary shapes and the exact analytical method. This figure also shows that the numerical calculation has an error of 0.06% relative to the analytical one.
Appendix C

L’Hôpital’s rule for stellar winds at the sonic point

The l’Hôpital’s rule gives us an expression for the first derivative of a function at a singular point.

Assume that the function $y(x)$ is described by the differential equation

$$\frac{dy(x)}{dx} = \frac{f(x)}{g(x)}. \quad (C.1)$$

The point $x = r_c$ is called a singular point of this function, when and only when $f(r_c) = g(r_c) = 0$. Then the derivative $dy(x)/dx$ can be developed by using the Taylor series expansion:

$$\left. \frac{dy}{dx} \right|_{r_c} = \frac{f(r_c) + \frac{x-r_c}{1!} f'(r_c) + \frac{(x-r_c)^2}{2!} f''(r_c) + ...}{g(r_c) + \frac{x-r_c}{1!} g'(r_c) + \frac{(x-r_c)^2}{2!} g''(r_c) + ...} \quad (C.2)$$

with the function $f(x)$ expanded at $r_c$ as

$$f(x) = f(r_c) + \frac{x-r_c}{1!} f'(r_c) + \frac{(x-r_c)^2}{2!} f''(r_c) + .... \quad (C.3)$$

Therefore, the first order differential Equation C.2 becomes

$$\left. \frac{dy}{dx} \right|_{r_c} = \frac{f'(r_c)}{g'(r_c)}. \quad (C.4)$$
If $f'(r_c)$ and $g'(r_c)$ are also equal to 0, one goes to the next order and a similar method gives us:

$$\frac{dy}{dx}\Big|_{r_c} = \frac{f''(r_c)}{g''(r_c)}. \quad (C.5)$$

This rule is very convenient to treat the velocity profile at the sonic point of stellar winds. The momentum equation in a stellar wind is usually formulated as:

$$\frac{1}{v} \frac{\partial v}{\partial r} = \left( \frac{2c_s^2}{r} - \frac{\partial c_s}{\partial r} - \frac{GM_*}{r^2} + f \right) / (v^2 - c_s^2) \quad (C.6)$$

where the function $f$ expresses the other forces acting on the gas, such as the radiation force from dust grains. At the sonic point $r_c$, the numerator and the denominator of this equation both equal to zeros, we thus apply the l'Hôpital’s law Equation C.4. Assuming constant sound speed, the application on Equation C gives us:

$$\left( \frac{1}{v} \frac{\partial v}{\partial r} \right)\Big|_{r_c} = \left[ -\frac{2c_s^2}{r_c^2} - \frac{\partial^2 c_s^2}{\partial^2 r} \Big|_{r_c} + 2GM_* \frac{r^3}{r_c^3} \frac{\partial}{\partial r} \Big|_{r_c} \right] / \left[ 2 \left( \frac{v}{\partial r} \right)\Big|_{r_c} \right] \quad (C.7)$$

with $v(r_c) = c_s$. Finally, the differential equation for the velocity of the stellar wind at $r_c$ is:

$$\frac{\partial v}{\partial r}\Big|_{r_c} = \sqrt{-\frac{c_s^2}{r_c} + \frac{GM_*}{r_c^3} - \frac{1}{2} \frac{\partial^2 c_s^2}{\partial^2 r} \Big|_{r_c} + \frac{1}{2} \frac{\partial f}{\partial r} \Big|_{r_c}}. \quad (C.8)$$

In practice, we use this rule whenever $0.99c_s < v_n < 1.01c_s$ and it allows us to go through the sonic point even in the cases where the numerator of does not vanish. We then adjust the starting velocity at the base of the wind so that this numerator is close to zero at the sonic point.
Appendix D

Motion of termination shock

In subsubsection 9.1.1.2 and subsubsection 9.2.1.2, the stellar wind velocity is computed in the star frame, while the termination shock velocity is considered in the shock frame. However, since we neglect the motion of the termination shock’s frame, we use the termination wind velocity as an input parameter for the termination shock. In this section, we will examine the relationship between the termination shock’s velocity in the shock frame and the terminal wind velocity in the star frame, which can infer the effect of the motion of the termination shock’s frame. The diagram of interaction between the stellar wind and the ISM is shown in Figure D.1.

In the termination shock’s frame, we call \( v_r \) the velocity of the termination shock and \( v_f \) the bow shock velocity. The balance of ram-pressure between both sides of the shock region gives us:

\[
\rho_w v_r^2 = \rho_a v_f^2 \tag{D.1}
\]

where \( \rho_w \) and \( \rho_a \) are the density of the inner wind region and the outer ISM ambient.

In the star’s frame, the terminal wind velocity (\( v_w \)) is:

\[
v_w = \Delta v_r + \Delta v_f \tag{D.2}
\]

where \( \Delta \) is the difference of the pre-shock velocity to the post-shock velocity. As indicated in Equation 4.38, the compression factor is \( 1/M^2 \) in the case of isothermal (\( \gamma = 1 \)), these differences are then:

\[
\Delta v_r = v_r - \frac{v_r}{M_r^2} \simeq v_r
\]

\[
\Delta v_f = v_f - \frac{v_r}{M_f^2} \simeq v_f \tag{D.3}
\]
where $M_r$ and $M_f$ are the Mach numbers of the reverse and the forward shocks. Substituting $v_f$ from Equation D.1 and Equation D.3, we get the relationship between $v_r$ and $v_w$ as:

$$v_r = \frac{v_w}{1 + \sqrt{\frac{\rho_o}{\rho_w}}}$$  \hspace{1cm} (D.4)

If $\rho_w \ll \rho_o$: $v_r = v_w$. Thus, the motion of the termination shock’s frame can be negligible. If $\rho_w \simeq \rho_o$: $v_r = v_w/2$. Thus, The termination shock’s frame moves at the velocity $u_s \simeq v_w/2$. If $\rho_w \gg \rho_o$: $v_r \simeq 0$. Thus, only forward shock occurs.
Appendix E

Calculation the specific intensity of the HI radiation from the detached shell

To calculate the specific intensity of the HI 21-cm line radiation (Equation 9.16), we need to calculate two integrations over the whole space.

Adopting the spherical symmetry of the CSE around star as in Figure E.1. At one point of a distance \( r_0 \) in the detached shell, we have:

\[
    r^2 = s^2 + r_0^2 \rightarrow s = \sqrt{r^2 - r_0^2}
\]  
(E.1)

where \( s \) is the coordinate along the line-of-sight. Therefore, the integrated specific intensity along one line-of-sight \( (r_0) \) is:

\[
    I_{v_r}(r_0) = e^{-\int_a^b k_{v_r}(\sqrt{s^2+r_0^2}) ds} \left( \int_a^b \epsilon_{v_r}(\sqrt{s^2+r_0^2}) e^{\int_a^s k_{v_r}(\sqrt{s'^2+r_0^2}) ds'} ds + \text{const.} \right). 
\]  
(E.2)

with \( a = -\sqrt{r^2 - r_0^2} \) and \( b = \sqrt{r^2 - r_0^2} \).

To verify our method, we took the radial physical profiles of temperature, velocity and density of Hoai et al. (2015) and computed the HI line profile in two cases of \( 10^{-7} \, M_{\odot} \, \text{yr}^{-1} \) and \( 10^{-5} \, M_{\odot} \, \text{yr}^{-1} \). Our results (Figure E.2) match well the figure (2) of Hoai et al. (2015), except at the central velocity.
FIGURE E.1: Spherical symmetry of the detached shell.
Figure E.2: HI line profiles of shells in free expansion for two mass loss rates with no background.
Appendix F

Table of $\text{H}_2$ rovibrational excitation levels
| $v=0, J$ | Energy (K) | $v=1, J$ | Energy (K) | $v=2, J$ | Energy (K) |
|---------|------------|---------|------------|---------|------------|
| 0       | 000.00     | 0       | 5987.1     | 0       | 11636      |
| 1       | 170.50     | 1       | 6149.2     | 1       | 11790      |
| 2       | 509.85     | 2       | 6471.6     | 2       | 12095      |
| 3       | 1015.2     | 3       | 6951.6     | 3       | 12551      |
| 4       | 1681.7     | 4       | 7584.6     | 4       | 13151      |
| 5       | 2503.9     | 5       | 8365.3     | 5       | 13891      |
| 6       | 3474.4     | 6       | 9286.6     | 6       | 14764      |
| 7       | 4586.4     | 7       | 10342      | 7       | 15763      |
| 8       | 5829.8     | 8       | 11522      | 8       | 16881      |
| 9       | 7197.0     | 9       | 12818      | 9       | 18107      |
| 10      | 8677.3     | 10      | 14221      | 10      | 19435      |
| 11      | 10262      | 11      | 15722      | 11      | 20854      |
| 12      | 11940      | 12      | 17311      | 12      | 22355      |
| 13      | 13703      | 13      | 18980      | 13      | 23931      |
| 14      | 15540      | 14      | 20718      | 14      | 25571      |
| 15      | 17444      | 15      | 22517      | 15      | 27266      |
| 16      | 19403      | 16      | 24368      | 16      | 29009      |
| 17      | 21412      | 17      | 26264      | 17      | 30792      |
| 18      | 23460      | 18      | 28195      | 18      | 32606      |
| 19      | 25540      | 19      | 30155      | 19      | 34445      |
| 20      | 27645      | 20      | 32135      | 20      | 36300      |
| 21      | 29767      | 21      | 34130      | 21      | 38165      |
| 22      | 31900      | 22      | 36131      |         |            |
| 23      | 34038      | 23      | 38134      |         |            |
| 24      | 36175      |         |            |         |            |
| 25      | 38305      |         |            |         |            |

**Table F.1:** Table of H$_2$ rovibrational excitation levels with $v = 0, 2$. 
| $v=3, J$ | Energy (K) | $v=4, J$ | Energy (K) | $v=5, J$ | Energy (K) |
|---------|------------|---------|------------|---------|------------|
| 0       | 16953      | 0       | 21943      | 0       | 26607      |
| 1       | 17098      | 1       | 22080      | 1       | 26736      |
| 2       | 17388      | 2       | 22353      | 2       | 26993      |
| 3       | 17819      | 3       | 22760      | 3       | 27375      |
| 4       | 18387      | 4       | 23296      | 4       | 27879      |
| 5       | 19086      | 5       | 23956      | 5       | 28499      |
| 6       | 19912      | 6       | 24734      | 6       | 29230      |
| 7       | 20857      | 7       | 25624      | 7       | 30064      |
| 8       | 21912      | 8       | 26617      | 8       | 30996      |
| 9       | 23070      | 9       | 27707      | 9       | 32016      |
| 10      | 24323      | 10      | 28884      | 10      | 33116      |
| 11      | 25660      | 11      | 30140      | 11      | 34290      |
| 12      | 27074      | 12      | 31467      | 12      | 35527      |
| 13      | 28557      | 13      | 32855      | 13      | 36820      |
| 14      | 30098      | 14      | 34297      | 14      | 38160      |
| 15      | 31690      | 15      | 35784      |         |            |
| 16      | 33325      | 16      | 37308      |         |            |
| 17      | 34994      | 17      | 38861      |         |            |
| 18      | 36690      |         |            |         |            |
| 19      | 38405      |         |            |         |            |

**Table F.2**: Table of H$_2$ rovibrational excitation levels with $v = 3, 5$.

| $v=6, J$ | Energy (K) | $v=7, J$ | Energy (K) | $v=8, J$ | Energy (K) |
|---------|------------|---------|------------|---------|------------|
| 0       | 30943      | 0       | 34946      | 0       | 38606      |
| 1       | 31064      | 1       | 35059      | 1       | 38709      |
| 2       | 31305      | 2       | 35282      | 2       | 38915      |
| 3       | 31662      | 3       | 35615      | 3       | 39221      |
| 4       | 32133      | 4       | 36052      |         |            |
| 5       | 32713      | 5       | 36590      |         |            |
| 6       | 33395      | 6       | 37222      |         |            |
| 7       | 34174      | 7       | 37943      |         |            |
| 8       | 35041      | 8       | 38744      |         |            |
| 9       | 35990      |         |            |         |            |
| 10      | 37013      |         |            |         |            |
| 11      | 38101      |         |            |         |            |

**Table F.3**: Table of H$_2$ rovibrational excitation levels with $v = 6, 8$. 
Appendix G

Input chemical species for the Paris-Durham shock code
| Name | Composition | Initial Density $n/n_H$ | Formation Enthalpy [kCal/mol] |
|------|-------------|-------------------------|-------------------------------|
| H    | 01000000000000 | 5.743D-06              | 51.634                        |
| H2   | 02000000000000 | 5.000D-01              | 0.00000                       |
| He   | 00000100000000 | 1.000D-01              | 0.00000                       |
| C    | 00500000000000 | 1.000D-15              | 169.980                       |
| CH   | 01010000000000 | 1.000D-15              | 141.600                       |
| CH2  | 02010000000000 | 1.000D-15              | 93.9000                       |
| CH3  | 03010000000000 | 1.000D-15              | 34.8000                       |
| CH4  | 04010000000000 | 1.000D-15              | -15.970                       |
| O    | 00001000000000 | 1.240D-04              | 58.9800                       |
| O2   | 01001000000000 | 1.000D-15              | 0.00000                       |
| OH   | 02001000000000 | 1.000D-15              | 57.100                        |
| CO   | 00010100000000 | 1.000D-15              | 27.200                        |
| CO2  | 00010200000000 | 1.000D-15              | 93.965                        |
| C2   | 00200000000000 | 1.000D-15              | 198.200                       |
| C2H  | 01020000000000 | 1.000D-15              | 113.300                       |
| C2H2 | 02020000000000 | 1.000D-15              | 56.3200                       |
| C3   | 00300000000000 | 1.000D-15              | 194.000                       |
| C3H  | 01030000000000 | 1.000D-15              | 177.000                       |
| C3H2 | 02030000000000 | 1.000D-15              | 114.000                       |
| CH3OH| 04010100000000 | 1.000D-15              | -99.999                       |
| CH2O | 02010100000000 | 1.000D-15              | -99.999                       |
| N    | 00010000000000 | 6.390D-05              | 112.530                       |
| NH   | 01001000000000 | 1.000D-15              | 90.00000                      |
| NH2  | 02001000000000 | 1.000D-15              | 46.2000                       |
| NH3  | 03001000000000 | 1.000D-15              | 9.2990                         |
| CN   | 00011000000000 | 1.000D-15              | 103.200                       |
| HCN  | 01011000000000 | 1.000D-15              | 32.3900                       |
| HNC  | 01011000000000 | 1.000D-15              | 48.0000                       |
| N2   | 00020000000000 | 1.000D-15              | 0.00000                       |
| NO   | 00011000000000 | 1.000D-15              | 21.4600                       |
| S    | 00000000010000 | 1.000D-15              | 65.6000                       |
| SH   | 01000000010000 | 1.000D-15              | 32.6000                       |
| H2S  | 02000000010000 | 1.000D-15              | 4.2300                        |
| CS   | 00010000010000 | 1.000D-15              | 63.0000                       |
| SO   | 00001000010000 | 1.000D-15              | 1.20000                       |
| SO2  | 00002000010000 | 1.000D-15              | -70.300                       |
| OCS  | 00010100010000 | 1.000D-15              | -34.000                       |
| Si   | 00000000001000 | 1.000D-15              | 106.700                       |
| SiH  | 01000000001000 | 1.000D-15              | 89.6900                       |
| SiH2 | 02000000001000 | 1.000D-15              | 69.1400                       |
| SiH3 | 03000000001000 | 1.000D-15              | 48.5400                       |
| Element  | Charge | Mass (amu) | Relative Abundance |
|----------|--------|-----------|-------------------|
| SiH4     | 0      | 0.00000000001000 | 1.000D-15           |
| SiO      | 0      | 0.00001000001000 | 1.000D-15           |
| SiO2     | 0      | 0.00002000001000 | 1.000D-15           |
| Mg       | 0      | 0.00000000100000 | 1.000D-15           |
| Fe       | 0      | 0.00000000000010 | 1.000D-15           |
| C54H18   | 1      | 1.85400000000000 | 1.000D-15           |
| G        | 0      | 0.00600000000000 | 2.107D-12           |
| H2O*     | 0      | 0.02000100000001 | 1.034D-04           |
| O2*      | 0      | 0.00000200000001 | 1.000D-15           |
| CO*      | 0      | 0.00001000000001 | 8.270D-06           |
| CO2*     | 0      | 0.00010200000001 | 1.340D-05           |
| CH4*     | 0      | 0.04010000000001 | 1.380D-06           |
| NH3*     | 0      | 0.03010000000001 | 1.550D-05           |
| N2*      | 0      | 0.00002000000001 | 1.000D-15           |
| CH3OH*   | 0      | 0.04010100000001 | 1.860D-05           |
| H2CO*    | 0      | 0.02010100000001 | 6.200D-06           |
| HCO2H*   | 0      | 0.02010200000001 | 7.240D-06           |
| OCS*     | 0      | 0.00010101000001 | 2.070D-07           |
| H2S*     | 0      | 0.00002000000001 | 1.000D-15           |
| Fe*      | 0      | 0.00000000000011 | 1.000D-15           |
| SiH4*    | 0      | 0.04000000001001 | 1.000D-15           |
| SiO*     | 0      | 0.00000100001001 | 1.000D-15           |
| SiO2*    | 0      | 0.00000200001001 | 1.000D-15           |
| O**      | 0      | 0.00001000000002 | 1.400D-04           |
| Si**     | 0      | 0.00000000001002 | 3.370D-05           |
| Mg**     | 0      | 0.00000000100002 | 3.700D-05           |
| Fe**     | 0      | 0.00000000000012 | 3.230D-05           |
| C**      | 0      | 0.00010000000002 | 1.630D-04           |
| H+       | 0      | 0.01000001000000 | 1.000D-15           |
| H2+      | 0      | 0.02000001000000 | 1.000D-15           |
| H3+      | 0      | 0.03000001000000 | 1.000D-15           |
| He+      | 0      | 0.00000011000000 | 1.000D-15           |
| C+       | 0      | 0.00010001000000 | 8.270D-05           |
| CH+      | 0      | 0.01010001000000 | 1.000D-15           |
| CH2+     | 0      | 0.02010001000000 | 1.000D-15           |
| CH3+     | 0      | 0.03010001000000 | 1.000D-15           |
| CH4+     | 0      | 0.04010001000000 | 1.000D-15           |
| CH5+     | 0      | 0.05010001000000 | 1.000D-15           |
| O+       | 0      | 0.00000101000000 | 1.000D-15           |
| O2+      | 0      | 0.00002001000000 | 1.000D-15           |
| OH+      | 0      | 0.01000101000000 | 1.000D-15           |
| H2O+     | 0      | 0.02000101000000 | 1.000D-15           |
| H3O+     | 0      | 0.03000101000000 | 1.000D-15           |
| CO+      | 0      | 0.00010101000000 | 1.000D-15           |
| HCO+     | 0      | 0.01010101000000 | 1.000D-15           |
| HCO2+    | 0      | 0.01010201000000 | 1.000D-15           |
| C2+      | 0      | 0.00020001000000 | 1.000D-15           |
| C2H+     | 0      | 0.01020001000000 | 1.000D-15           |
| C2H2+    | 0      | 0.02020001000000 | 1.000D-15           |
| C2H3+    | 0      | 0.03020001000000 | 1.000D-15           |
| No. | Species     | Ions     | Charge   | Energy (kJ/mol) | Temperature (K) |
|-----|-------------|----------|----------|----------------|-----------------|
| 70  | C3+        | 00030001000000 | 1.000D-15 | 479.000       | *               |
| 71  | C3H+       | 01030001000000 | 1.000D-15 | 381.000       | *               |
| 72  | C3H2+      | 02030001000000 | 1.000D-15 | 330.000       | * **            |
| 73  | C3H3+      | 03030001000000 | 1.000D-15 | 282.000       | * **            |
| 74  | N+         | 00011001000000 | 1.000D-15 | 447.690       |                 |
| 75  | NH+        | 01011001000000 | 1.000D-15 | 401.100       |                 |
| 76  | NH2+       | 02011001000000 | 1.000D-15 | 302.700       | **              |
| 77  | NH3+       | 03011001000000 | 1.000D-15 | 284.000       | **              |
| 78  | NH4+       | 04011001000000 | 1.000D-15 | 226.000       | **              |
| 79  | CN+        | 00011001000000 | 1.000D-15 | 429.300       | **              |
| 80  | C2N+       | 00021001000000 | 1.000D-15 | 410.000       | **              |
| 81  | HCN+       | 01011001000000 | 1.000D-15 | 346.000       |                 |
| 82  | H2CN+      | 02011001000000 | 1.000D-15 | 237.000       | **              |
| 83  | H2NC+      | 03011001000000 | 1.000D-15 | 265.000       | **              |
| 84  | N2+        | 00020010000000 | 1.000D-15 | 359.298       |                 |
| 85  | N2H+       | 01020010000000 | 1.000D-15 | 247.500       |                 |
| 86  | NO+        | 00011001000000 | 1.000D-15 | 235.330       |                 |
| 87  | HNO+       | 01011001000000 | 1.000D-15 | 256.800       | **              |
| 88  | S+         | 00000001010000 | 1.470D-05 | 304.000       | **              |
| 89  | SH+        | 01000001010000 | 1.000D-15 | 271.800       | **              |
| 90  | H2S+       | 02000001010000 | 1.000D-15 | 237.000       | **              |
| 91  | H3S+       | 03000001010000 | 1.000D-15 | 190.000       | **              |
| 92  | CS+        | 00010001010000 | 1.000D-15 | 324.000       | **              |
| 93  | HCS+       | 01010001010000 | 1.000D-15 | 243.000       | **              |
| 94  | SO+        | 00000010101000 | 1.000D-15 | 239.200       | **              |
| 95  | HSO+       | 01000101010000 | 1.000D-15 | 210.000       | **              |
| 96  | HSO2+      | 01000201010000 | 1.000D-15 | 143.000       | **              |
| 97  | HOC+       | 01010101010000 | 1.000D-15 | 181.000       | **              |
| 98  | Si+        | 00000001010000 | 1.000D-15 | 295.000       | **              |
| 99  | SiH+       | 01000001010000 | 1.000D-15 | 271.820       | **              |
| 100 | SiH2+      | 02000001010000 | 1.000D-15 | 276.360       | **              |
| 101 | SiH3+      | 03000001010000 | 1.000D-15 | 237.320       | **              |
| 102 | SiH4+      | 04000001010000 | 1.000D-15 | 239.280       | **              |
| 103 | SiH5+      | 05000001010000 | 1.000D-15 | 219.380       | **              |
| 104 | SiO+       | 00000001010000 | 1.000D-15 | 239.520       | **              |
| 105 | SiOH+      | 01000001010000 | 1.000D-15 | 295.000       | **              |
| 106 | Fe+        | 00000001010000 | 1.500D-08 | 280.240       | **              |

**Table G.1:** List of input chemical species for the Paris-Durham shock code.
Appendix H

Full chemical network for the Paris-Durham shock code

Note this is the network we used for the interstellar bow-shock computations, and it does not include the three-body reactions described in subsection 8.4.2.
Appendix H

columns:

* reference or comment
* R1, R2, P1, P2, P3, P4 : reactants and product of the reaction
  R1 + R2 -> P1 + P2 + P3 + P4
* gamma(cm^3.s^-1), beta(K), alpha : Ahrrenius coefficients

in general :
  rate = gamma*EXP(-beta/T)*(T/300)**alpha

special cases :
* photo-reactions
  rate = gamma*EXP(-beta*Av)*RAD
* CR induced desorption from grains
  rate = gamma*sigma(grain)*N(grains)/N(species on grains)
* CR ionisation or dissociation
  rate = gamma*EXP(-beta/T)*(T/300)**alpha + other terms...
* H2 and HD formation
  rate = gamma*(T/300)**alpha*nH/n(H)
* three body reactions on grains surface
  rate = gamma*<sigma.v>(grain)*N(grains)/N(species on grains)
  /(Teff/beta+1)**
* sputtering of grain mantle
  complicated!
* erosion of grain cores
  rate = gamma*EXP(-beta/T)*(T/300)**alpha * <sigma.v>(grain)
* adsorption on grains
  rate = gamma*<sigma.v>(grain)

| R1 | R2 | P1 | P2 | P3 | P4 | gamma | alpha | beta |
|----|----|----|----|----|----|-------|-------|------|
|     |     |     |     |     |     | 8.14D-17 | 0.5   |      |
| B7  | 88  | H   | H2  |     |     | 9.20D-10 | 0.5  | 157890.0 |
| IONIZ H | +ELECTR =H+ | ELECTR | ELECTR | 1.40D-00 | 0.5 | 179160.0 |
| IONIZ H | +H+ =H+ | H+ | ELECTR | 1.30D-13 | 0.5 | 157890.0 |
| IONIZ H | +H3+ =H3+ | H+ | ELECTR | 1.30D-13 | 0.5 | 157890.0 |
| IONIZ H | +He+ =He+ | H+ | ELECTR | 1.30D-13 | 0.5 | 157890.0 |
| IONIZ H | +H3O+ =H3O+ | H+ | ELECTR | 1.30D-13 | 0.5 | 157890.0 |
| IONIZ H | +H3S+ =H3S+ | H+ | ELECTR | 1.30D-13 | 0.5 | 157890.0 |
| IONIZ H | +HCO+ =HCO+ | H+ | ELECTR | 1.30D-13 | 0.5 | 157890.0 |
| IONIZ H | +Fe+ =Fe+ | H+ | ELECTR | 1.30D-13 | 0.5 | 157890.0 |
| IONIZ H | +NH3+ =NH3+ | H+ | ELECTR | 1.30D-13 | 0.5 | 157890.0 |
| IONIZ H | +NH4+ =NH4+ | H+ | ELECTR | 1.30D-13 | 0.5 | 157890.0 |
| IONIZ H | +S+ =S+ | H+ | ELECTR | 1.30D-13 | 0.5 | 157890.0 |
| IONIZ H | +SiOH+ =SiOH+ | H+ | ELECTR | 1.30D-13 | 0.5 | 157890.0 |
| IONIZ H | +O2+ =O2+ | H+ | ELECTR | 1.30D-13 | 0.5 | 157890.0 |
| IONIZ H | +H+ =H+ | H2 | ELECTR | 1.10D-13 | 0.5 | 179160.0 |
| IONIZ H | +H3+ =H3+ | H2 | ELECTR | 1.10D-13 | 0.5 | 179160.0 |
| IONIZ H | +He+ =He+ | H2 | ELECTR | 1.10D-13 | 0.5 | 179160.0 |
| IONIZ H | +H3O+ =H3O+ | H2 | ELECTR | 1.10D-13 | 0.5 | 179160.0 |
| IONIZ H | +H3S+ =H3S+ | H2 | ELECTR | 1.10D-13 | 0.5 | 179160.0 |
| IONIZ H | +HCO+ =HCO+ | H2 | ELECTR | 1.10D-13 | 0.5 | 179160.0 |
| IONIZ H | +He+ =He+ | H2 | ELECTR | 1.10D-13 | 0.5 | 179160.0 |
| IONIZ H | +H3O+ =H3O+ | H2 | ELECTR | 1.10D-13 | 0.5 | 179160.0 |
| IONIZ H | +H3S+ =H3S+ | H2 | ELECTR | 1.10D-13 | 0.5 | 179160.0 |
| IONIZ H | +HCO+ =HCO+ | H2 | ELECTR | 1.10D-13 | 0.5 | 179160.0 |
| IONIZ H | +Fe+ =Fe+ | H2 | ELECTR | 1.10D-13 | 0.5 | 179160.0 |
| IONIZ H | +NH3+ =NH3+ | H2 | ELECTR | 1.10D-13 | 0.5 | 179160.0 |
| IONIZ H | +NH4+ =NH4+ | H2 | ELECTR | 1.10D-13 | 0.5 | 179160.0 |
| IONIZ H | +S+ =S+ | H2 | ELECTR | 1.10D-13 | 0.5 | 179160.0 |
| IONIZ H | +SiOH+ =SiOH+ | H2 | ELECTR | 1.10D-13 | 0.5 | 179160.0 |
| IONIZ H | +O2+ =O2+ | H2 | ELECTR | 1.10D-13 | 0.5 | 179160.0 |
| IONIZ H | +H+ =H+ | He+ | ELECTR | 1.10D-13 | 0.5 | 285328.0 |
| IONIZ H | +H3+ =H3+ | He+ | ELECTR | 1.10D-13 | 0.5 | 285328.0 |
| IONIZ H | +He+ =He+ | He+ | ELECTR | 1.10D-13 | 0.5 | 285328.0 |
| IONIZ H | +H3O+ =H3O+ | He+ | ELECTR | 1.10D-13 | 0.5 | 285328.0 |
| IONIZ H | +H3S+ =H3S+ | He+ | ELECTR | 1.10D-13 | 0.5 | 285328.0 |
| IONIZ H | +HCO+ =HCO+ | He+ | ELECTR | 1.10D-13 | 0.5 | 285328.0 |
| IONIZ H | +Fe+ =Fe+ | He+ | ELECTR | 1.10D-13 | 0.5 | 285328.0 |
| IONIZ H | +NH3+ =NH3+ | He+ | ELECTR | 1.10D-13 | 0.5 | 285328.0 |

---------------------------------------------
IONIZ He  +NH4+  =NH4+  He+  ELECTR  1.10D-13  0.5  285328.0
IONIZ He  +S+  =S+  He+  ELECTR  1.10D-13  0.5  285328.0
IONIZ He  +SiOH+  =SiOH+  He+  ELECTR  1.10D-13  0.5  285328.0
IONIZ He  +O2+  =O2+  He+  ELECTR  1.10D-13  0.5  285328.0
DISSO H2  +ELECTR =ELECTR  H       H              2.00D-09  0.5  116300.0
DISSO H2  +H      =H       H       H              3.99D-07  -1.03  52000.0
DISSO H2  +He     =He      H       H              1.00D-11  0.0   52000.0
DISSO H2  +H2     =H2      H       H              4.98D-08  -1.03  52000.0
DISSO H2  +H+     =H+      H       H              3.00D-11  0.5   52000.0
DISSO H2  +H3+    =H3+     H       H              3.00D-11  0.5   52000.0
DISSO H2  +He+    =He+     H       H              3.00D-11  0.5   52000.0
DISSO H2  +H3O+   =H3O+    H       H              3.00D-11  0.5   52000.0
DISSO H2  +H3S+   =H3S+    H       H              3.00D-11  0.5   52000.0
DISSO H2  +HCO+   =HCO+    H       H              3.00D-11  0.5   52000.0
DISSO H2  +Fe+    =Fe+     H       H              3.00D-11  0.5   52000.0
DISSO H2  +NH3+   =NH3+    H       H              3.00D-11  0.5   52000.0
DISSO H2  +NH4+   =NH4+    H       H              3.00D-11  0.5   52000.0
DISSO H2  +S+     =S+      H       H              3.00D-11  0.5   52000.0
DISSO H2  +SiOH+  =SiOH+   H       H              3.00D-11  0.5   52000.0
DISSO H2  +O2+    =O2+     H       H              3.00D-11  0.5   52000.0
D&B   H2     +PHOTON =H       H                      2.54D-11  0.00     0.00
lee   CO     +PHOTON =C       O                      1.03D-10  0.00     0.00
TYPE2 C      +PHOTON =C+      ELECTR                 2.20E-10  0.00     2.96
12z88 CH      PHOTON  C       H                      9.50E-10  0.00     1.1
12z88 CH      PHOTON  CH+     ELECTR                 7.60E-10  0.00     2.8
12z88 CH2    PHOTON  CH       H                      7.20E-10  0.00     1.7
36b77 CH2    PHOTON  CH2+    ELECTR                 3.00E-10  0.00     2.3
12z88 CH3    PHOTON  CH3     H                      5.00E-10  0.00     1.9
36b77 CH3    PHOTON  CH3+    ELECTR                 1.00E-10  0.00     2.1
12z88 CH4    PHOTON  CH4     H2                     1.20E-09  0.00     2.1
12z88 OH     PHOTON  OH      H                      8.00E-10  0.00     1.7
12z88 H2O    PHOTON  OH      H2                     8.00E-10  0.00     1.7
12z88 H2O    PHOTON  H2O+    ELECTR                 3.30E-11  0.00     3.9
12z88 H2O    PHOTON  H2O     H                       3.00E-10  0.00     1.7
12z88 H2O    PHOTON  H2      H2                     5.00E-10  0.00     1.7
12z88 H2O    PHOTON  H2      H       H              5.00E-10  0.00     1.7
12z88 H2O    PHOTON  H2      H       H              5.00E-10  0.00     1.7
UMIST CH3OH  PHOTON  H2CO    H2                     6.00E-10  0.00     1.8
UMIST CH3OH  PHOTON  OH      CH3                    6.00E-10  0.00     1.8
UMIST H2CO   PHOTON  CO      H6                     7.00E-10  0.00     1.7
UMIST H2CO   PHOTON  H6O+    ELECTR                 1.40E-11  0.00     3.1
12z88 NH     PHOTON  N       H                      5.00E-10  0.00     1.8
12z88 NH     PHOTON  NH+     ELECTR                 1.00E-11  0.00     2.0
12z88 NH2    PHOTON  NH       H                      7.40E-10  0.00     1.6
12z88 NH2    PHOTON  NH2+    ELECTR                 1.73E-10  0.00     2.6
12z88 NH3    PHOTON  NH3     H                      1.10E-09  0.00     1.8
12z88 NH3    PHOTON  NH3+    ELECTR                 2.80E-10  0.00     2.7
12z88 CN     PHOTON  CN       H                      3.00E-10  0.00     3.1
12z88 HCN    PHOTON  CN       H                      1.50E-09  0.00     2.1
12z88 HNC    PHOTON  CN       H                      1.50E-09  0.00     2.1
12z88 N2     PHOTON  N       H                      2.30E-10  0.00     3.8
12z88 NO     PHOTON  N       0                      4.70E-10  0.00     1.7
12z88 NO     PHOTON  NO+     ELECTR                 2.60E-10  0.00     2.3
12z88 S      PHOTON  S       H                      5.90E-10  0.00     2.6
12z88 SH     PHOTON  S       H                      9.70E-10  0.00     1.4
| Species | Process | Product | Charge | Energy (eV) | Width (meV) |
|---------|---------|---------|--------|------------|-------------|
| 12z88 H2S | PHOTON H2S+ | ELECTR | 7.10E-10 | 0.00 | 2.7 |
| 12z88 H2S | PHOTON SH | H | 3.10E-09 | 0.00 | 1.9 |
| 12z88 C5 | PHOTON C S | 9.70E-10 | 0.00 | 2.0 |
| 12z88 S0 | PHOTON S 0 | 3.70E-09 | 0.00 | 1.9 |
| 12z88 S02 | PHOTON S0 0 | 1.90E-09 | 0.00 | 1.9 |
| 12z88 OCS | PHOTON S0 | CO | 3.70E-09 | 0.00 | 1.7 |
| St&Da Si | +PHOTON =Si+ | ELECTR | 7.10E-10 | 0.00 | 2.55 |
| St&Da SiH | +PHOTON =Si | H | 1.50E-09 | 0.00 | 2.55 |
| guess SiH3 | +PHOTON =SiH2 | H | 1.50E-09 | 0.00 | 2.55 |
| guess SiH4 | +PHOTON =SiH3 | H | 1.50E-09 | 0.00 | 2.55 |
| St&Da SiO | +PHOTON =SiO+ | ELECTR | 5.00E-11 | 0.00 | 2.55 |
| guess Si | +PHOTON =SiH | H | 1.50E-09 | 0.00 | 2.55 |
| guess Si+ | +PHOTON =SiH2 | H2 | 1.50E-09 | 0.00 | 2.55 |
| 12z88 Fe | PHOTON Fe+ | ELECTR | 2.80E-10 | 0.00 | 1.9 |
| 12z88 H2+ | PHOTON H+ | H | 5.70E-10 | 0.00 | 1.9 |
| 35 87 H3+ | PHOTON H2+ | H | 5.00E-13 | 0.00 | 2.3 |
| 35 87 H3+ | PHOTON H+ | H2 | 5.00E-13 | 0.00 | 1.8 |
| 15 88 CH+ | PHOTON H+ | C | 1.00E-10 | 0.00 | 1.7 |
| guess NH2+ | PHOTON =N+ | H2 | 1.00E-10 | 0.00 | 2.0 |
| guess NH3+ | PHOTON NH+ | H2 | 1.00E-10 | 0.00 | 2.0 |
| guess NH4+ | PHOTON NH3+ | H | 1.00E-10 | 0.00 | 2.0 |
| guess CN+ | PHOTON C+ | N | 1.00E-10 | 0.00 | 2.0 |
| guess C2N+ | PHOTON CN+ | C | 1.00E-10 | 0.00 | 2.0 |
| guess HCN+ | PHOTON HCN+ | H | 1.00E-10 | 0.00 | 2.0 |
| guess N2+ | PHOTON N+ | N | 1.00E-10 | 0.00 | 2.0 |
| guess N2H+ | PHOTON N+ | H2 | 1.00E-10 | 0.00 | 2.0 |
| guess NH3+ | PHOTON NH+ | H2 | 1.00E-10 | 0.00 | 2.0 |
| guess NH4+ | PHOTON NH3+ | H | 1.00E-10 | 0.00 | 2.0 |
| guess CN+ | PHOTON C+ | N | 1.00E-10 | 0.00 | 2.0 |
| guess C2N+ | PHOTON CN+ | C | 1.00E-10 | 0.00 | 2.0 |
| guess HCN+ | PHOTON HCN+ | H | 1.00E-10 | 0.00 | 2.0 |
| guess N2+ | PHOTON N+ | N | 1.00E-10 | 0.00 | 2.0 |
| guess N2H+ | PHOTON N+ | H2 | 1.00E-10 | 0.00 | 2.0 |
| guess NH3+ | PHOTON NH+ | H2 | 1.00E-10 | 0.00 | 2.0 |
| guess NH4+ | PHOTON NH3+ | H | 1.00E-10 | 0.00 | 2.0 |
| guess CN+ | PHOTON C+ | N | 1.00E-10 | 0.00 | 2.0 |
| guess C2N+ | PHOTON CN+ | C | 1.00E-10 | 0.00 | 2.0 |
| guess HCN+ | PHOTON HCN+ | H | 1.00E-10 | 0.00 | 2.0 |
| guess N2+ | PHOTON N+ | N | 1.00E-10 | 0.00 | 2.0 |
| guess N2H+ | PHOTON N+ | H2 | 1.00E-10 | 0.00 | 2.0 |
| guess NH3+ | PHOTON NH+ | H2 | 1.00E-10 | 0.00 | 2.0 |
| guess NH4+ | PHOTON NH3+ | H | 1.00E-10 | 0.00 | 2.0 |
| guess CN+ | PHOTON C+ | N | 1.00E-10 | 0.00 | 2.0 |
| Reaction | Products | Cooling Type | Cooling Value | Temp. Value |
|----------|----------|--------------|---------------|-------------|
| guess HS02+ + PHOTON = HS0+ | 1.00E-10 | 0.00 | 2.0 |
| guess HOC5+ + PHOTON = CS+ | 1.00E-10 | 0.00 | 2.0 |
| Guess SiH+ + PHOTON = SiH+ | 1.00E-09 | 0.00 | 2.55 |
| Guess SiH2+ + PHOTON = SiH2+ | 1.00E-09 | 0.00 | 2.55 |
| Guess SiH3+ + PHOTON = SiH3+ | 1.00E-09 | 0.00 | 2.55 |
| Guess SiH4+ + PHOTON = SiH4+ | 1.00E-09 | 0.00 | 2.55 |
| Guess SiH5+ + PHOTON = SiH5+ | 1.00E-09 | 0.00 | 2.55 |
| St&Da SiO+ + PHOTON = Si+ | 1.50E-11 | 0.00 | 2.55 |
| St&Da SiOH+ + PHOTON = SiO+ | 1.50E-11 | 0.00 | 2.55 |
| C54H18 + ELECTR = C54H18- | 1.00E-07 | 0.00 | 0.0 |
| C54H18++ELECTR = C54H18 | 3.30E-06 | -0.50 | 0.0 |
| C54H18++C54H18- = C54H18 | 3.00E-09 | -0.50 | 0.0 |
| C54H18-+H+ = C54H18 | 7.50E-08 | -0.50 | 0.0 |
| C54H18-+H3+ = C54H18 | 2.20D-08 | -0.50 | 0.0 |
| C54H18-+H3+ = C54H18 | 2.20D-08 | -0.50 | 0.0 |
| C54H18-+He+ = C54H18 | 3.80D-08 | -0.50 | 0.0 |
| C54H18-+C+ = C54H18 | 2.20D-08 | -0.50 | 0.0 |
| C54H18-+H3O+ = C54H18 | 1.70D-08 | -0.50 | 0.0 |
| C54H18-+H3S+ = C54H18 | 1.30D-08 | -0.50 | 0.0 |
| C54H18-+NH4+ = C54H18 | 1.80D-08 | -0.50 | 0.0 |
| C54H18-+HCO+ = C54H18 | 1.40E-08 | -0.50 | 0.0 |
| C54H18-+HCS+ = C54H18 | 1.10D-08 | -0.50 | 0.0 |
| C54H18-+H2CN+ = C54H18 | 1.10D-08 | -0.50 | 0.0 |
| C54H18-+Si+ = C54H18 | 1.40D-08 | -0.50 | 0.0 |
| C54H18-+Fe+ = C54H18 | 1.40D-08 | -0.50 | 0.0 |
| C54H18-+S+ = C54H18 | 1.40D-08 | -0.50 | 0.0 |
| C54H18-+H = C54H18 | 4.40D-09 | 0.00 | 0.0 |
| C54H18-+C = C54H18 | 9.60D-10 | 0.00 | 5500.0 |
| C54H18-+CH = C54H18 | 9.60D-10 | 0.00 | 5500.0 |
| C54H18-+O = C54H18 | 8.30D-10 | 0.00 | 5500.0 |
| C54H18-+OH = C54H18 | 8.30D-10 | 0.00 | 5500.0 |
| C54H18-+SECPHO = C54H18+ | 1.00E-08 | 0.00 | 140000.0 |
| C54H18-+SECPHO = C54H18- | 2.00E+04 | 0.00 | 140000.0 |
| P & H H + CRP = H+ | 4.60E-01 | 0.00 | 0.0 |
| P & H He + CRP = H+ | 5.00E-01 | 0.00 | 0.0 |
| P & H H2 + CRP = H+ | 4.00E-02 | 0.00 | 0.0 |
| P & H H2 + CRP = H+ | 1.50E-06 | 0.00 | 0.0 |
| P & H C + CRP = C+ | 9.60E-01 | 0.00 | 0.0 |
| P & H O + CRP = O+ | 1.80E+00 | 0.00 | 0.0 |
| P & H O + CRP = O+ | 2.80E+00 | 0.00 | 0.0 |
| 56 88 C + SECPHO = C+ | 1.02E+02 | 0.00 | 140000.0 |
| 2Z89 CH + SECPHO = C+ | 1.46E+03 | 0.00 | 140000.0 |
| 13 87 CH4 + SECPHO = CH3 | 4.68E+03 | 0.00 | 140000.0 |
| 2Z89 CH+ + SECPHO = C+ | 3.52E+02 | 0.00 | 140000.0 |
| 2Z89 OH + SECPHO = H | 1.02E+03 | 0.00 | 140000.0 |
| 2Z89 H2O + SECPHO = OH | 1.94E+03 | 0.00 | 140000.0 |
| 2Z89 O2 + SECPHO = O2+ | 2.34E+02 | 0.00 | 140000.0 |
| 2Z89 O2 + SECPHO = O2+ | 1.50E+03 | 0.00 | 140000.0 |
| 2Z89 C02 + SECPHO = C0 | 3.42E+03 | 0.00 | 140000.0 |
| 2Z89 C2 + SECPHO = C2 | 4.74E+02 | 0.00 | 140000.0 |
| 77 87 C2H + SECPHO = C2 | 8.16E+03 | 0.00 | 140000.0 |
| 2Z89 C2H2 + SECPHO = C2H | 1.03E+04 | 0.00 | 140000.0 |
Appendix H

2289 C2H2 +SECPhO =C2H2+ ELECTR  2.62D+03  0.00  140000.0
2288 C3 +SECPhO =C2 C  2.24D+03  0.00  140000.0
13 87 C3H +SECPhO =C3 H  8.16D+03  0.00  140000.0
13 87 C3H2 +SECPhO =C3H H  8.16D+03  0.00  140000.0
56 88 C0 +SECPhO =C0  6.80D+02  1.20  140000.0
16883 O +H2 =OH H  1.55D-13  2.80  2980.0
UMIST C0 +H =OH C  1.10D-10  -.90  8770.0
72 83 O2 +H =OH O  1.63D-09  -.90  8770.0
16883 OH +H =H2O H  7.00D-14  2.00  1490.0
16883 H2O +H =OH H2  5.24D-12  1.90  9265.0
17B73 C +H2 =CH H2  1.16D-09  0.50  14100.0
P & H C +H =CH PHOTON  1.00D-17  0.00  0.0
22 86 CH +H2 =CH2 H2  2.38D-10  0.00  1760.0
17B73 CH2 +H2 =CH3 H2  5.18D-11  0.17  6400.0
23 86 CH3 +H2 =CH4 H2  3.00D-10  0.00  5460.0
59 82 C2 +H2 =C2H H2  1.60D-10  0.00  1419.0
S88 C2H +H2 =C2H2 H2  1.14D-11  0.00  950.0
17B73 CH +H =C H2  1.16D-09  0.50  2200.0
22 86 CH2 +H =CH H2  4.70D-10  0.00  370.0
17B73 CH3 +H =CH2 H2  5.18D-11  0.17  5600.0
23863 CH4 +H =CH3 H2  3.00D-10  0.00  6560.0
P & H O2 +C =CO O  3.30D-11  0.50  0.0
93 88 OH +CO =CO2 H  4.40D-13 -1.15  390.0
95 88 OH +C =CO O  3.10D-11  -.36  0.0
61 81 CH +O =HCO+ ELECTR  2.40D-14  0.50  0.0
61 81 CH +O =CO O  9.50D-11  0.50  0.0
P & H CH2 +O =CO O  2.00D-10  0.00  4827.0
14 87 CH+ +H =CH+ H  1.50D-10  0.00  4827.0
14 87 CH+ +O =CO+ O  9.50D-11  0.50  0.0
27877 CH+ +H2 =CH2+ H  1.20D-09  0.00  0.0
27877 CH2+ +H+ =CH+ H2  1.20D-09  0.00  2790.0
28875 CH2+ +H2 =CH3+ H  7.00D-10  0.00  0.0
28875 CH3+ +H =CH2+ H2  7.00D-10  0.00  10560.0
4289 CH3+ +H2 =CH5+ PHOTON  6.00D-15  0.00  0.0
28875 CH3+ +H2 =CH4+ H  2.00D-10  0.00  32500.0
28875 CH4+ +H =CH3+ H2  2.00D-10  0.00  0.0
28875 CH4+ +H2 =CH5+ H2  4.00D-11  0.00  2200.0
28875 CH5+ +H =CH4+ H2  4.00D-11  0.00  2200.0
H+ +ELECTR =H PHOTON  2.90D-12 -1.74  0.0
22290 H2+ +ELECTR =H H  1.60D-08 -1.43  0.0
P & H He+ +ELECTR =He ELECTR  4.50D-12 -1.67  0.0
McC03 H3+ ELECTR H H H  5.10D-08 -1.52  0.0
McC03 H3+ ELECTR H2 H  1.70D-08 -1.52  0.0
P & H C+ +ELECTR =C PHOTON  4.40D-12 -1.61  0.0
22290 CH+ +ELECTR =C H  1.50D-07 -1.42  0.0
22290 CH2+ +ELECTR =C2 H2  1.25D-07 -1.50  0.0
22290 CH2+ +ELECTR =CH H  1.25D-07 -1.50  0.0
22290 CH3+ +ELECTR =CH2 H  1.75D-07 -1.50  0.0
22290 CH3+ +ELECTR =CH H2  1.75D-07 -1.50  0.0
P & H CH4+ +ELECTR =CH4 H H  3.00D-07 -1.50  0.0
P & H CH4+ +ELECTR =CH2 H H  3.00D-07 -1.50  0.0
22290 CH5+ +ELECTR =CH H2 H2  8.75D-08 -1.30  0.0
22290 CH5+ +ELECTR =CH2 H2  8.75D-08 -1.30  0.0
22290 CH5+ +ELECTR =CH3 H2  8.75D-08 -1.30  0.0
22290 CH5+ +ELECTR =CH4 H  8.75D-08 -1.30  0.0
79 79 H+ +H2 =H2+ H  6.40D-10  0.00  21300.0
| Reaction | Stoichiometry | Energy | Internal Energy | Temperature |
|----------|---------------|--------|----------------|-------------|
| 01R79 H₂⁺ +H =H⁺ + H₂ | +6.40D-10 | 0.00 | 0.0 | 227.0 |
| P & H H₂⁺ +H₂ =H₃⁺ + H₂ | +2.10D-09 | 0.00 | 0.0 | 20600.0 |
| 52R84 H⁺ +O =O⁺ + H | +6.00D-10 | 0.00 | 0.0 | 227.0 |
| P & H H₂⁺ +H₂ =H₃⁺ + H₂ | +2.10D-09 | 0.00 | 0.0 | 20600.0 |
| P & H H⁺ +CH =CH⁺ + H₂ | +1.90D-09 | 0.00 | 0.0 | 20000.0 |
| P & H H⁺ +CH₂ =CH⁺ + H₂ | +1.40D-09 | 0.00 | 0.0 | 20000.0 |
| P & H H⁺ +CH₃ =CH₃⁺ + H₂ | +3.40D-09 | 0.00 | 0.0 | 20000.0 |
| P & H H⁺ +CH₄ =CH₃⁺ + H₂ | +2.28D-09 | 0.00 | 0.0 | 20000.0 |
| P & H H⁺ +O₂ =O₂⁺ + H | +8.20D-09 | 0.00 | 0.0 | 20000.0 |
| 80R74 H⁺ +O₂ =O₂⁺ + H | +1.20D-09 | 0.00 | 0.0 | 20000.0 |
| 80R74 H⁺ +H₂O =H₂O⁺ + H | +1.52D-09 | 0.00 | 0.0 | 20000.0 |
| P & H H⁺ +CH =CH⁺ + H | +1.90D-09 | 0.00 | 0.0 | 20000.0 |
| P & H H⁺ +CH₂ =CH₂⁺ + H | +1.40D-09 | 0.00 | 0.0 | 20000.0 |
| P & H H⁺ +CH₃ =CH₃⁺ + H₂ | +1.00D-09 | 0.00 | 0.0 | 20000.0 |
| P & H H⁺ +CH₄ =CH₄⁺ + H | +1.52D-09 | 0.00 | 0.0 | 20000.0 |
| 38R75 H₂⁺ +CO =HCO⁺ + H | +2.16D-09 | 0.00 | 0.0 | 20000.0 |
| P & H H₂⁺ +C =CH⁺ + H | +2.40D-09 | 0.00 | 0.0 | 20000.0 |
| P & H H₂⁺ +O =OH⁺ + H | +1.50D-09 | 0.00 | 0.0 | 20000.0 |
| 38R75 H₂⁺ +CO =CO⁺ + H | +6.44D-10 | 0.00 | 0.0 | 20000.0 |
| 52R89 H₃⁺ +CO =HCO⁺ + H | +1.00D-09 | 0.00 | 0.0 | 20000.0 |
| 80R82 H₃⁺ +CO₂ =HCO₂⁺ + H | +2.00D-09 | 0.00 | 0.0 | 20000.0 |
| 40R75 H₃⁺ +H₂O =H₃O⁺ + H | +4.30D-09 | 0.00 | 0.0 | 20000.0 |
| P & H H₃⁺ +C =CH⁺ + H | +2.00D-09 | 0.00 | 0.0 | 20000.0 |
| P & H H₃⁺ +CH =CH₂⁺ + H | +1.20D-09 | 0.00 | 0.0 | 20000.0 |
| P & H H₃⁺ +CH₂ =CH₃⁺ + H | +1.70D-09 | 0.00 | 0.0 | 20000.0 |
| P & H H₃⁺ +CH₃ =CH₄⁺ + H | +2.10D-09 | 0.00 | 0.0 | 20000.0 |
| 52B89 H₃⁺ +CH₄ =CH₅⁺ + H | +1.90D-09 | 0.00 | 0.0 | 20000.0 |
| 5Z89 He⁺ +H₂ =H⁺ + H | +1.10D-13 | -.24 | 0.0 | 20000.0 |
| P & H He⁺ +OH =OH⁺ + He | +5.50D-10 | 0.00 | 0.0 | 20000.0 |
| 38R76 He⁺ +CO =C⁺ + O | +1.50D-09 | 0.00 | 0.0 | 20000.0 |
| 81R77 He⁺ +CO₂ =CO⁺ + O₂ | +4.00D-11 | 0.00 | 0.0 | 20000.0 |
| P & H He⁺ +CH =C⁺ + H | +1.10D-09 | 0.00 | 0.0 | 20000.0 |
| P & H He⁺ +CH₂ =C⁺ + H | +7.50D-10 | 0.00 | 0.0 | 20000.0 |
| 43R76 He⁺ +CH₄ =C⁺ + CH₃ | +4.00D-10 | 0.00 | 0.0 | 20000.0 |
| 43R76 He⁺ +CH₄ =CH₂⁺ + H | +2.56D-10 | 0.00 | 0.0 | 20000.0 |
| 43R76 He⁺ +CH₄ =CH₃⁺ + H | +8.40D-10 | 0.00 | 0.0 | 20000.0 |
| 43R76 He⁺ +CH₄ =CH₄⁺ | +8.00D-11 | 0.00 | 0.0 | 20000.0 |
| 88 B5 C⁺ +OH =CO⁺ | +8.00D-10 | 0.00 | 0.0 | 20000.0 |
| 88 B5 C⁺ +OH =H⁺ + CO | +8.00D-10 | 0.00 | 0.0 | 20000.0 |
| 74B85 C⁺ +H₂O =HCO⁺ | +2.43D-09 | -.63 | 0.0 | 20000.0 |
| 73R84 C⁺ +CO₂ =CO⁺ + O₂ | +3.15D-10 | 0.00 | 0.0 | 20000.0 |
| 82R81 C⁺ +CO₂ =CO⁺ + O₂ | +1.00D-09 | 0.00 | 0.0 | 20000.0 |
| 78 B3 C⁺ +CH =C⁺ + H | +3.80D-10 | 0.00 | 0.0 | 20000.0 |
| P & H C⁺ +CH₂ =CH²⁺ | +3.00D-10 | 0.00 | 0.0 | 20000.0 |
| P & H C⁺ +CH₂ =CH₃⁺ | +5.20D-10 | 0.00 | 0.0 | 20000.0 |
| P & H C⁺ +CH₃ =CH₄⁺ | +5.20D-10 | 0.00 | 0.0 | 20000.0 |
| Reaction | Products | Rate Constant | E (eV) | A (cm³/mol/s) |
|----------|----------|---------------|-------|--------------|
| 7R82 C⁺ + CH₄ → C₂H₂ + H₂ | 3.25×10⁻¹⁰ | 0.00 | 0.0 |
| 52R84 O⁺ + CH₄ → C₂H₃⁺ + H | 6.00×10⁻¹⁰ | 0.00 | 0.0 |
| P & H O₂⁺ + H⁺ → O⁺ + H₂ | 1.20×10⁻⁹ | 0.00 | 0.0 |
| P & H O₂⁺ + C⁺ → C₂H₂⁺ + H₂ | 5.20×10⁻¹¹ | 0.00 | 0.0 |
| 44R81 OH⁺ + H₂O → C₂H₂⁺ + H | 9.75×10⁻⁹ | 0.00 | 0.0 |
| 52R84 O⁺ + H₂ → OH⁺ + H | 1.80×10⁻¹⁰ | 0.00 | 0.0 |
| P & H H₃O⁺ + H⁺ → H₂O⁺ + H₂ | 6.00×10⁻¹⁰ | 0.00 | 20500.0 |
| P & H H₃O⁺ + CH₂⁺ → CH₃⁺ + H₂O | 1.00×10⁻¹⁰ | 0.00 | 0.0 |
| P & H O⁺ + ELECTRON → O⁺ + PHOTON | 3.40×10⁻¹² | -.64 | 0.0 |
| 1Z83 O₂⁺ + ELECTRON → O⁺ + H₂ | 1.95×10⁻⁷ | -.70 | 0.0 |
| 22Z90 OH⁺ + ELECTRON → O⁺ + H | 3.75×10⁻⁸ | -.50 | 0.0 |
| 44R81 H₂O⁺ + ELECTRON → H⁺ + H₂ | 3.15×10⁻⁷ | -.50 | 0.0 |
| 90 88 H₃O⁺ + ELECTRON → H₂O⁺ + H₂ | 8.45×10⁻⁷ | -.50 | 0.0 |
| 49R76 CH₃⁺ + O⁺ → H⁺ + CO | 1.30×10⁻¹² | 0.00 | 0.0 |
| 51R80 CH₅⁺ + O₂ → H⁺ + CH₂ | 2.16×10⁻¹⁰ | 0.00 | 0.0 |
| 8R80 CH₅⁺ + O₂ → H⁺ + CH₂ | 1.40×10⁻¹⁰ | 0.00 | 0.0 |
| 40R75 CH₅⁺ + H₂O → H⁺ + CH₃ | 7.50×10⁻⁸ | 0.00 | 9060.0 |
| 49R76 CH₃⁺ + O₂ → H⁺ + CO₂ | 1.30×10⁻¹⁰ | 0.00 | 0.0 |
| 46C84 CH₃⁺ + H₂O → H⁺ + CH₄ | 5.00×10⁻¹⁰ | 0.00 | 800.0 |
| 8R80 CH₅⁺ + H₂O → H⁺ + CH₃ | 2.16×10⁻¹⁰ | 0.00 | 0.0 |
| 22Z90 CH₂⁺ + ELECTRON → C⁺ | 3.00×10⁻⁷ | -.50 | 0.0 |
| 22Z90 CH₂⁺ + ELECTRON → C₂⁺ | 1.50×10⁻⁷ | -.50 | 0.0 |
| 6Z88 CH₂⁺ + ELECTRON → C₂H⁺ | 1.50×10⁻⁷ | -.50 | 0.0 |
| 46C84 CH₂⁺ + H₂O → H⁺ + CH₃ | 1.50×10⁻⁷ | 0.00 | 0.0 |
| 65R78 H₂O⁺ + H₂O → H₂O⁺ + H₂ | 2.50×10⁻⁹ | 0.00 | 0.0 |
| 15 H⁺ + O₂ → H⁺ + CO₂ | 1.00×10⁻⁹ | 0.00 | 1450.0 |
| 15 H⁺ + O₂ → H⁺ + CO₂ | 1.00×10⁻⁹ | 0.00 | 0.0 |
| 15 H⁺ + O₂ → H⁺ + CO₂ | 1.00×10⁻⁹ | 0.00 | 5000.0 |
| 75 88 C₂H₂⁺ + ELECTRON → C₂H⁺ | 1.50×10⁻⁷ | -.50 | 0.0 |
| 75 88 C₂H₂⁺ + ELECTRON → C₂H₂⁺ | 1.50×10⁻⁷ | -.50 | 0.0 |
| 75 88 C₂H₂⁺ + ELECTRON → C₂H₂⁺ | 3.00×10⁻⁸ | -.50 | 0.0 |
| 58 83 C⁺ + H₂ → C⁺ + H₂ | 3.00×10⁻⁹ | 0.00 | 0.0 |
| 62 86 C⁺ + H₂ → C₂H⁺ | 3.00×10⁻¹³ | -1.0 | 0.0 |
| 46C84 C₂H⁺ + ELECTRON → C₂H₂⁺ | 3.00×10⁻⁷ | -.50 | 0.0 |
| 8R80 CH₃⁺ + H₂O → H⁺ + C₂H₃⁺ | 1.00×10⁻⁸ | 0.00 | 0.0 |
| 52R84 O⁺ + H₂ → O⁺ + H₂ | 7.50×10⁻¹⁰ | 0.00 | 0.0 |
| Reaction | Products | Energy | Temperature |
|----------|----------|--------|-------------|
| P & H H+ + C2 = C2+ H | 3.10D-09 | 0.00 | 0.0 |
| P & H H+ + C2H = C2+ H2 | 1.50D-09 | 0.00 | 0.0 |
| 78 83 H+ + C2H2 = C2H+ H2 | 2.00D-09 | 0.00 | 0.0 |
| 84 83 H+ + C3H = C3H+ H | 2.00D-09 | 0.00 | 0.0 |
| 84 83 H+ + C3H2 = C3H2+ H | 2.00D-09 | 0.00 | 0.0 |
| 78 83 H+ + C2H2 = C2H+ H2 | 2.00D-09 | 0.00 | 0.0 |
| P & H H+ + C2H = C2H+ H | 1.50D-09 | 0.00 | 0.0 |
| 78 83 H+ + C2H2 = C2H+ H2 | 2.00D-09 | 0.00 | 0.0 |
| 84 83 H+ + C3H = C3H+ H | 2.00D-09 | 0.00 | 0.0 |
| 84 83 H+ + C3H2 = C3H2+ H | 2.00D-09 | 0.00 | 0.0 |
| 78 83 H+ + C2H2 = C2H+ H2 | 2.00D-09 | 0.00 | 0.0 |
| P & H H+ + C2H = C2H+ H | 1.50D-09 | 0.00 | 0.0 |
| 78 83 H+ + C2H2 = C2H+ H2 | 2.00D-09 | 0.00 | 0.0 |
| 84 83 H+ + C3H = C3H+ H | 2.00D-09 | 0.00 | 0.0 |
| 84 83 H+ + C3H2 = C3H2+ H | 2.00D-09 | 0.00 | 0.0 |
| 78 83 H+ + C2H2 = C2H+ H2 | 2.00D-09 | 0.00 | 0.0 |
| P & H H+ + C2H = C2H+ H | 1.50D-09 | 0.00 | 0.0 |
| 78 83 H+ + C2H2 = C2H+ H2 | 2.00D-09 | 0.00 | 0.0 |
| 84 83 H+ + C3H = C3H+ H | 2.00D-09 | 0.00 | 0.0 |
| 84 83 H+ + C3H2 = C3H2+ H | 2.00D-09 | 0.00 | 0.0 |
| 78 83 H+ + C2H2 = C2H+ H2 | 2.00D-09 | 0.00 | 0.0 |
| P & H H+ + C2H = C2H+ H | 1.50D-09 | 0.00 | 0.0 |
| 78 83 H+ + C2H2 = C2H+ H2 | 2.00D-09 | 0.00 | 0.0 |
| 84 83 H+ + C3H = C3H+ H | 2.00D-09 | 0.00 | 0.0 |
| 84 83 H+ + C3H2 = C3H2+ H | 2.00D-09 | 0.00 | 0.0 |
| 78 83 H+ + C2H2 = C2H+ H2 | 2.00D-09 | 0.00 | 0.0 |
| P & H H+ + C2H = C2H+ H | 1.50D-09 | 0.00 | 0.0 |
| 78 83 H+ + C2H2 = C2H+ H2 | 2.00D-09 | 0.00 | 0.0 |
| 84 83 H+ + C3H = C3H+ H | 2.00D-09 | 0.00 | 0.0 |
| 84 83 H+ + C3H2 = C3H2+ H | 2.00D-09 | 0.00 | 0.0 |
| 78 83 H+ + C2H2 = C2H+ H2 | 2.00D-09 | 0.00 | 0.0 |
|   |   |   |     |  |   |
|---|---|---|-----|---|---|
| 97 83 NH3 | OH | NH2 | H2O | 2.30D-12 | 0.00 | 800.0 |
| P & H NH | C | CN | H | 1.10D-10 | 0.50 | 0.0 |
| 94 88 CH | N | CN | H | 2.10D-11 | 0.00 | 0.0 |
| 97 83 CN+ | N | N2 | C | 7.30D-10 | 0.00 | 4500.0 |
| P & H NH | N | N2 | H | 5.00D-11 | 0.50 | 0.0 |
| 94E88 OH | N | N0 | H | 5.30D-11 | 0.00 | 50.0 |
| 97 83 O2 | N | NO | O | 3.30D-12 | 1.00 | 3150.0 |
| P & H NO | C | CN | O | 1.10D-10 | 0.50 | 0.0 |
| 94E88 O2 | N | NO | O | 3.40D-11 | 0.00 | 50.0 |
| 94 88 CH | N | N2 | H | 2.10D-11 | 0.00 | 0.0 |
| 97 83 CN | N | N2 | C | 7.30D-10 | 0.00 | 4500.0 |
| P & H NH | N | N2 | H | 5.00D-11 | 0.50 | 0.0 |
| 94E88 OH | N | N0 | H | 5.30D-11 | 0.00 | 50.0 |
| 97 83 O2 | N | NO | H | 3.30D-12 | 1.00 | 3150.0 |
| P & H NO | C | CN | O | 1.10D-10 | 0.50 | 0.0 |
| 94E88 O2 | N | NO | O | 3.40D-11 | 0.00 | 50.0 |
| 94 88 CH | N | N2 | H | 2.10D-11 | 0.00 | 0.0 |
| 97 83 CN | N | N2 | C | 7.30D-10 | 0.00 | 4500.0 |
| P & H NH | N | N2 | H | 5.00D-11 | 0.50 | 0.0 |
| 94E88 OH | N | N0 | H | 5.30D-11 | 0.00 | 50.0 |
| 97 83 O2 | N | NO | O | 3.30D-12 | 1.00 | 3150.0 |
| P & H NO | C | CN | O | 1.10D-10 | 0.50 | 0.0 |
| 94E88 O2 | N | NO | O | 3.40D-11 | 0.00 | 50.0 |

Appendix H
| Reaction | Left Side | Right Side | Energy | Oscillator | Comment |
|----------|-----------|-----------|--------|------------|---------|
| P & H H3+ | CN | H2CN+ H | 1.000-09 | 0.00 | 0.0 |
| 12R85 H3+ | HCN | H2CN+ H2 | 9.500-09 | 0.00 | 0.0 |
| 12R85 H3+ | HNC | H2CN+ H2 | 9.500-09 | 0.00 | 0.0 |
| 5Z89 H3+ | N2 | N2H+ H2 | 1.300-09 | 0.00 | 0.0 |
| 08R82 H3+ | NO | HNO+ H2 | 1.100-09 | 0.00 | 0.0 |
| 19R80 H30+ | NH3 | HNH+ H2O | 2.200-09 | 0.00 | 0.0 |
| H30+ | CN | H2CN+ OH | 4.500-09 | 0.00 | 0.0 |
| 19R78 H30+ | HCN | H2CN+ H2O | 4.500-09 | 0.00 | 2460.0 |
| 19R78 H2CN+ | H2O | H30+ HCN | 4.500-09 | 0.00 | 0.0 |
| 19R78 H30+ | HNC | H2CN+ H2O | 4.500-09 | 0.00 | 0.0 |
| 19R78 H2CN+ | H2O | H30+ HCN | 4.500-09 | 0.00 | 10300.0 |
| P & H HCO+ | NH | NH2+ CO | 6.400-10 | 0.00 | 0.0 |
| P & H NH2+ | CO | H2O+ H | 6.400-10 | 0.00 | 6100.0 |
| P & H HCO+ | NH2 | NH3+ CO | 8.900-10 | 0.00 | 0.0 |
| 05R78 HCO+ | NO | HNO+ CO2 | 1.900-10 | 0.00 | 0.0 |
| P & H C+ | NH | CN+ H | 7.800-10 | 0.00 | 0.0 |
| P & H C+ | NH2 | HCN+ H | 1.100-09 | 0.00 | 0.0 |
| 05R79 C+ | NH3 | NH3+ C | 5.200-10 | 0.00 | 0.0 |
| 05R79 C+ | NH3 | H2NC+ | 7.800-10 | 0.00 | 0.0 |
| 05R79 C+ | NH3 | H2CN+ | 7.800-10 | 0.00 | 0.0 |
| 05R79 C+ | NH3 | HCN+ | 7.800-10 | 0.00 | 0.0 |
| 05R79 C+ | NO | NO+ CO2 | 3.400-09 | 0.00 | 0.0 |
| P & H C+ | NH3 | NH4+ CO2 | 1.700-09 | 0.00 | 0.0 |
| 12R85 C+ | HCN | C2N+ H | 3.400-09 | 0.00 | 0.0 |
| 12R85 C+ | HNC | C2N+ H | 3.400-09 | 0.00 | 0.0 |
| 09R84 C+ | NO | NO+ C | 3.400-09 | 0.00 | 0.0 |
| 09R84 C+ | NO | NO+ CO2 | 9.020-10 | 0.00 | 0.0 |
| 09R84 N+ | CO | CO+ N | 9.020-10 | 0.00 | 15400.0 |
| 17R77 O2+ | N | O2+ N | 7.840-11 | 0.00 | 0.0 |
| 18R83 O2+ | NO | NO+ O2 | 4.400-10 | 0.00 | 0.0 |
| P & H CH2+ | N | HCN+ H | 9.400-10 | 0.00 | 0.0 |
| P & H C2H+ | N | C2N+ H | 8.300-10 | 0.00 | 0.0 |
| P & H CH3+ | N | HCN+ H2 | 6.700-11 | 0.00 | 0.0 |
| M88 CH3+ | N | H2CN+ H | 6.700-11 | 0.00 | 0.0 |
| M88 C2H2+ | N | CH+ HCN | 2.500-11 | 0.00 | 0.0 |
| M88 C2H2+ | N | CH+ HNC | 2.500-11 | 0.00 | 2600.0 |
| M88 C2H2+ | N | C2N+ H2 | 2.250-10 | 0.00 | 0.0 |
| 17R80 N+ | O2 | O2+ N | 2.810-10 | 0.00 | 0.0 |
| 17R80 N+ | O2 | NO+ O | 2.370-10 | 0.00 | 0.0 |
| 17R80 N+ | O2 | O+ N | 3.300-11 | 0.00 | 0.0 |
| 08R84 N+ | CO | CO+ N | 8.250-10 | 0.00 | 0.0 |
| 08R84 N+ | CO | NO+ C | 1.460-10 | 0.00 | 0.0 |
| 10R80 N+ | NO | NO+ N | 4.510-10 | 0.00 | 0.0 |
| 10R80 N+ | NO | N2+ O | 7.950-11 | 0.00 | 0.0 |
| 13R83 NH3+ | H2O | NH4+ OH | 2.500-10 | 0.00 | 3480.0 |
| 13R83 NH4+ | OH | NH3+ H2O | 2.500-10 | 0.00 | 3480.0 |
| 06R80 N2H+ | O | OH+ N2 | 1.400-10 | 0.00 | 3480.0 |
| 06R80 N2H+ | CO | HCO+ N2 | 8.800-10 | 0.00 | 0.0 |
| 06R80 HCO+ | N2 | H2O+ C2H2 | 8.800-10 | 0.00 | 11200.0 |
| 08R82 N2H+ | CO2 | HCO2+ N2 | 1.400-09 | 0.00 | 0.0 |
| 08R82 HCO2+ | N2 | N2H+ CO2 | 1.400-09 | 0.00 | 6400.0 |
| 15R74 N2H+ | NH3 | NH4+ N2 | 2.300-09 | 0.00 | 0.0 |
| 15R74 NH4+ | N2 | N2H+ NH3 | 2.300-09 | 0.00 | 44600.0 |
| 08R82 N2H+ | NO | HNO+ N2 | 3.400-10 | 0.00 | 0.0 |
| 01R83 C2N+ | NH3 | N2H+ C2H2 | 1.900-10 | 0.00 | 0.0 |
| 01R83 C2N+ | NH3 | H2CN+ HCN | 1.700-09 | 0.00 | 0.0 |
| P & H HNO+ | C | CH+ NO | 1.000-09 | 0.00 | 0.0 |
| 04R71 HNO+ | CO | HCO+ N2 | 1.000-10 | 0.00 | 0.0 |
| 04R71 HNO+ | CO2 | HCO2+ N2 | 1.000-10 | 0.00 | 0.0 |
| P & H HNO+ | OH | H2O+ N2 | 6.200-10 | 0.00 | 0.0 |
| 08R82 HNO+ | H2O | H3O+ NO | 2.300-09 | 0.00 | 0.0 |
| P & H NO+ | Fe | Fe+ NO | 1.000-09 | 0.00 | 0.0 |
| P & H N+ | ELECTR | N PHOTON | 3.800-12 | -0.62 | 0.0 |
| P & H NH+ | ELECTR | N | H | 2.00D-07 -0.50 0.0 |
|-----------|---------|---|---|-------------------|
| P & H NH2+| ELECTR | NH | H | 1.50D-07 -0.50 0.0 |
| P & H NH2+| ELECTR | N | H | 1.50D-07 -0.50 0.0 |
| 22290 NH3+| ELECTR | NH2 | H | 3.00D-07 -0.50 0.0 |
| 22290 NH4+| ELECTR | NH2 | H2 | 7.60D-07 -0.50 0.0 |
| 22290 NH4+| ELECTR | NH3 | H | 7.60D-07 -0.50 0.0 |
| P & H CN+ | ELECTR | C | N | 1.80D-07 -0.50 0.0 |
| 75 88 C2N+ | ELECTR | C2 | N | 1.00D-07 -0.50 0.0 |
| 75 88 C2N+ | ELECTR | CN | C | 2.00D-07 -0.50 0.0 |
| 75 88 HCN+ | ELECTR | CN | H | 1.50D-07 -0.50 0.0 |
| 75 88 HCN+ | ELECTR | CH | N | 1.50D-07 -0.50 0.0 |
| 22290 N2+ | ELECTR | N | N | 3.60D-08 -0.42 0.0 |
| 6Z88 N2H+ | ELECTR | N2 | H | 1.70D-07 -1.00 0.0 |
| 7Z88 H2CN+ | ELECTR | HCN | H | 1.75D-07 -0.50 0.0 |
| 7Z88 H2CN+ | ELECTR | HNC | H | 1.75D-07 -0.50 0.0 |
| 7Z88 H2NC+ | ELECTR | HNC | H | 1.75D-07 -0.50 0.0 |
| 7Z88 H2NC+ | ELECTR | NH2 | C | 1.75D-07 -0.50 0.0 |
| 22290 NO+ | ELECTR | N | O | 4.30D-07 -0.37 0.0 |
| P & H HNO+ | ELECTR | NO | H | 3.00D-07 -0.50 0.0 |
| 15 88 SO | +SECPHO =S | O | 9.64D+02 0.00 140000.0 |
| 15 88 CS | +SECPHO =S | C | 2.12D+04 0.00 140000.0 |
| 15 88 SH | +SECPHO =S | H | 1.46D+03 0.00 140000.0 |
| 2Z89 OCS | +SECPHO =CO | S | 1.07D+04 0.00 140000.0 |
| 2Z89 H2S | +SECPHO =S | H2 | 1.03D+04 0.00 140000.0 |
| 23Z90 NO | +SECPHO =SO | O | 1.77D+03 0.00 140000.0 |
| 16Z88 S | +H2 =SH | H | 1.04D-10 .132 9620.0 |
| 16Z88 SH | +H2 =H2S | H | 6.41D-12 .087 8050.0 |
| 16Z88 SH | +H =S | H2 | 2.50D-11 0.00 860.0 |
| 16Z88 SO | +H =S | O2 | 6.60D-13 0.00 2760.0 |
| 16Z88 SO | +O =S | OH | 5.97D-12 -.31 11100.0 |
| 16Z88 SO | +O2 =S | O | 5.19D-12 0.00 2650.0 |
| UMIST SH | +S =SH | H2 | 1.00D-10 0.00 100.0 |
| 17288 SH | +OH =SH | H2 | 1.70D-11 0.00 2650.0 |
| 17288 SH | +SH =H2S | H | 1.04D-11 .132 9620.0 |
| 17288 SH | +H =S | H2 | 6.30D-12 0.00 80.0 |
| 16Z88 C5 | +S =C5 | S | 2.70D-10 0.00 760.0 |
| 16Z88 C5 | +OH =C5S | H | 1.55D-13 1.12 800.0 |
| 24Z87 S | +OH =SH | H2 | 5.19D-12 0.00 2650.0 |
| 16Z88 SO | +S =SO | O2 | 6.60D-13 0.00 2760.0 |
| 16Z88 SO | +O =SO | 02 | 1.40D-12 0.00 2820.0 |
| UMIST SO | +C =SO | S | 1.73D-11 0.50 750.0 |
| 16Z88 SO | +C =SO | S | 7.20D-11 0.00 0.0 |
| 16Z88 SO | +S =SO | H2 | 1.00D-11 0.00 100.0 |
| 16Z88 SO | +O =SO | H2O | 9.27D-11 -.46 9140.0 |
| 16Z88 SH | +S =SH | H2O | 2.60D-11 0.00 2250.0 |
| 16Z88 CH | +S =SH | C | 1.10D-12 0.00 0.0 |
| 16Z88 CH | +C =SH | H | 1.73D-11 0.50 4000.0 |
| 16Z88 CH | +H =S+ | H | 1.00D-10 0.00 100.0 |
| 16Z88 SH | +C =SH | H2 | 2.00D-11 0.00 0.0 |
| 16Z88 SH | +C =CH | S | 1.20D-11 0.58 5880.0 |
| 16Z88 SH | +S =SH | OH | 5.95D-14 1.12 8330.0 |
| 18286 H2S+ | +H2 =SH | H2 | 2.20D-10 0.00 9860.0 |
| 18286 H2S+ | +H2 =H2S+ | H2 | 1.90D-10 0.00 8590.0 |
| P & H H+ | +S =S+ | PHOTON | 1.00D-15 0.00 0.0 |
| 18286 H2S+ | +H2 =H2S+ | H | 1.40D-11 0.00 2300.0 |
| 18286 H2S+ | +H2 =H2S+ | H2 | 6.00D-11 0.00 0.0 |
| GUESS H+ | +S =S+ | H | 1.00D-15 0.00 0.0 |
| P & H H+ | +SH =SH | H | 1.60D-09 0.00 0.0 |
| P & H H+ | +SH =S+ | H2 | 1.60D-09 0.00 0.0 |
| Reaction                  | Products  | Ea (kJ/mol) | DeltaG (kJ/mol) | DeltaS (kJ/mol) |
|--------------------------|-----------|-------------|-----------------|-----------------|
| \( \text{P \& H H} + \text{H}_{2}\text{S} \rightarrow \text{H}_{2}\text{S} + \text{H} \) |           | 7.60E-09    | 0.00            | 0.0             |
| \( \text{P \& H H} + \text{CS} \rightarrow \text{CS} + \text{H} \) |           | 4.90E-09    | 0.00            | 0.0             |
| \( \text{P \& H H} + \text{SO} \rightarrow \text{SO} + \text{H} \) |           | 3.20E-09    | 0.00            | 0.0             |
| \( \text{P \& H H} + \text{OCS} \rightarrow \text{SH} + \text{CO} \) |           | 5.19E-09    | 0.00            | 0.0             |
| \( \text{P \& H H} + \text{S} \rightarrow \text{SH} + \text{H}_2 \) |           | 3.46E-09    | 0.00            | 0.0             |
| \( \text{P \& H H} + \text{SH} \rightarrow \text{H}_{2}\text{S} + \text{H} \) |           | 2.94E-09    | 0.00            | 0.0             |
| \( \text{P \& H H} + \text{H}_{2}\text{S} \rightarrow \text{H}_{3}\text{S} + \text{H} \) |           | 1.96E-09    | 0.00            | 0.0             |
| \( \text{P \& H H} + \text{CS} \rightarrow \text{HCS} + \text{H}_2 \) |           | 2.66E-09    | 0.00            | 0.0             |
| \( \text{P \& H H} + \text{SO} \rightarrow \text{HSO} + \text{H}_2 \) |           | 1.85E-09    | 0.00            | 0.0             |
| \( \text{P \& H He} + \text{SH} \rightarrow \text{S} + \text{H} \) |           | 1.70E-09    | 0.00            | 0.0             |
| \( \text{P \& H He} + \text{H}_{2}\text{S} \rightarrow \text{S} + \text{H}_2 \) |           | 3.60E-09    | 0.00            | 0.0             |
| \( \text{P \& H He} + \text{H}_{2}\text{S} \rightarrow \text{SH} + \text{H} \) |           | 4.80E-10    | 0.00            | 0.0             |
| \( \text{P \& H He} + \text{H}_{2}\text{S} \rightarrow \text{H}_{2}\text{S} + \text{He} \) |           | 3.10E-10    | 0.00            | 0.0             |
| \( \text{P \& H He} + \text{CS} \rightarrow \text{C} + \text{S} \) |           | 1.30E-09    | 0.00            | 0.0             |
| \( \text{P \& H He} + \text{CS} \rightarrow \text{S} + \text{C} \) |           | 1.30E-09    | 0.00            | 0.0             |
| \( \text{P \& H He} + \text{SO} \rightarrow \text{S} + \text{O} \) |           | 8.30E-10    | 0.00            | 0.0             |
| \( \text{P \& H He} + \text{SO} \rightarrow \text{S} + \text{O} \) |           | 8.30E-10    | 0.00            | 0.0             |
| \( \text{P \& H He} + \text{OCS} \rightarrow \text{CS} + \text{O} \) |           | 7.60E-10    | 0.00            | 0.0             |
| \( \text{P \& H He} + \text{OCS} \rightarrow \text{S} + \text{CO} \) |           | 7.60E-10    | 0.00            | 0.0             |
| \( \text{P \& H He} + \text{OCS} \rightarrow \text{O} + \text{CS} \) |           | 7.60E-11    | 0.00            | 0.0             |
| \( \text{P \& H C} + \text{SO}_2 \rightarrow \text{SO} + \text{O}_2 \) |           | 8.60E-10    | 0.00            | 0.0             |
| \( \text{P \& H C} + \text{SO}_2 \rightarrow \text{SO} + \text{O} \) |           | 3.44E-09    | 0.00            | 0.0             |
| \( \text{P \& H C} + \text{S} \rightarrow \text{S} + \text{C} \) |           | 4.00E-09    | 0.00            | 0.0             |
| \( \text{P \& H C} + \text{S} \rightarrow \text{S} + \text{C} \) |           | 4.00E-09    | 0.00            | 0.0             |
| \( \text{P \& H C} + \text{CS} \rightarrow \text{CS} + \text{C} \) |           | 1.60E-09    | 0.00            | 7.00            |
| \( \text{P \& H C} + \text{SO} \rightarrow \text{SO} + \text{CO} \) |           | 2.60E-10    | 0.00            | 0.0             |
| \( \text{P \& H C} + \text{SO} \rightarrow \text{CO} + \text{S} \) |           | 2.60E-10    | 0.00            | 0.0             |
| \( \text{P \& H C} + \text{OCS} \rightarrow \text{OCS} + \text{CO} \) |           | 2.60E-10    | 0.00            | 0.0             |
| \( \text{P \& H C} + \text{OCS} \rightarrow \text{O} + \text{CS} \) |           | 2.60E-10    | 0.00            | 0.0             |
| \( \text{P \& H C} + \text{S} \rightarrow \text{S} + \text{C} \) |           | 6.20E-10    | 0.00            | 0.0             |
| \( \text{P \& H C} + \text{S} \rightarrow \text{S} + \text{C} \) |           | 6.20E-10    | 0.00            | 0.0             |
| \( \text{P \& H C} + \text{S} \rightarrow \text{S} + \text{C} \) |           | 6.20E-10    | 0.00            | 0.0             |
| Reaction   | Products     | Reaction   | Products     |
|------------|--------------|------------|--------------|
| 28875 SiH2+ | H2           | SiH3+     | H            |
| 28875 SiH3+ | H2           | SiH4+     | H            |
| 2570 SiH4+  | H2           | SiH5+     | H            |
| 27877 SiH2+ | H2           | SiH3+     | H            |
| 28875 SiH3+ | H2           | SiH4+     | H            |
| 28875 SiH4+ | H2           | SiH5+     | H            |
| 2791 SiO+   | H2           | SiOH+     | H            |
| 2570 SiH2+  | H2           | SiH3+     | H            |
| 28875 SiH3+ | H2           | SiH4+     | H            |
| 28875 SiH4+ | H2           | SiH5+     | H            |
| 2791 SiO+   | H2           | SiOH+     | H            |
| 411 H+      | SiH+         | Si+       | H2           |
| 412 H+      | SiH+         | Si+       | H2           |
| 420 H+      | SiH2+        | Si+       | H2           |
| 425 H+      | SiH3+        | Si+       | H2           |
| 426 H+      | SiH3+        | Si+       | H2           |
| 429 H+      | SiH4+        | Si+       | H2           |
| 430 H+      | SiH4+        | Si+       | H2           |
| 461 H+      | SiO+         | Si+       | O+           |
| 411 H+      | SiH+         | Si+       | H2           |
| 412 H+      | SiH+         | Si+       | H2           |
| 420 H+      | SiH2+        | Si+       | H2           |
| 425 H+      | SiH3+        | Si+       | H2           |
| 426 H+      | SiH3+        | Si+       | H2           |
| 429 H+      | SiH4+        | Si+       | H2           |
| 430 H+      | SiH4+        | Si+       | H2           |
| 461 H+      | SiO+         | Si+       | O+           |
| 411 H+      | SiH+         | Si+       | H2           |
| 412 H+      | SiH+         | Si+       | H2           |
| 420 H+      | SiH2+        | Si+       | H2           |
| 425 H+      | SiH3+        | Si+       | H2           |
| 426 H+      | SiH3+        | Si+       | H2           |
| 429 H+      | SiH4+        | Si+       | H2           |
| 430 H+      | SiH4+        | Si+       | H2           |
| 461 H+      | SiO+         | Si+       | O+           |
| 1033 C+     | Si+          | Si+       | C            |
| 1072 C+     | SiH2+        | Si+       | C            |
| 1125 C+     | SiO+         | Si+       | C            |
| 2471 S+     | Si+          | Si+       | S            |
| 2489 S+     | SiH+         | Si+       | H            |
| 618 H3+     | Si+          | Si+       | H2           |
| 644 H3+     | SiH2+        | Si+       | H2           |
| 648 H3+     | SiH2+        | Si+       | H2           |
| 652 H3+     | SiH2+        | Si+       | H2           |
| 654 H3+     | SiH4+        | Si+       | H2           |
| 680 H3+     | SiO+         | Si+       | H2           |
| 1731 H3O+   | Si+          | Si+       | H2           |
| 1745 H3O+   | SiH2+        | Si+       | H2           |
| 1746 H3O+   | SiH2+        | Si+       | H2           |
| 1764 H3O+   | SiH2+        | Si+       | H2           |
| 2258 HCO+   | Si+          | Si+       | C            |
| 2279 HCO+   | SiH+         | Si+       | C            |
| 2283 HCO+   | SiH2+        | Si+       | C            |
| 2286 HCO+   | SiH4+        | Si+       | C            |
| 2305 HCO+   | SiO+         | Si+       | C            |
| 2567 Si+    | SiO+         | Si+       | H2           |
| 2882 Si+    | O2           | SiO+      | H2           |
| 2226 SiH+   | O2           | SiO+      | H2           |
| 2229 SiH+   | NH3          | NH4+      | Si            |
| 2230 SiH+   | H3O+         | H3O+      | Si            |
| 2391 SiH2+  | O2           | SiO+      | H2           |
| 2393 SiH2+  | O2           | SiO+      | H2           |
| 2458 SiH+   | O2           | SiO+      | H2           |
| 2571 SiH4+  | CO           | HCO+      | SiH3          |
| 2572 SiH4+  | CO           | HCO+      | SiH3          |
| 2623 SiH5+  | CO           | HCO+      | SiH3          |

**Appendix H 175**
| Mass  | Species  | Charge  | Species  | Charge  | Mass  | Species  | Charge  | Species  | Charge  |
|-------|----------|---------|----------|---------|-------|----------|---------|----------|---------|
| 3116  | Si+      | ELECTR  | Si       | PHOTON  | 4.90E-12 | -0.60 | 0.0      | 3125  | SiH+     | ELECTR  | Si       | H       | 2.00E-07 | -0.50 | 0.0      |
| 3135  | SiH2+    | ELECTR  | Si       | H       | 2.00E-07 | -0.50 | 0.0      | 3136  | SiH2+    | ELECTR  | SiH     | H       | 1.50E-07 | -0.50 | 0.0      |
| 3146  | SiH3+    | ELECTR  | SiH2    | H       | 1.50E-07 | -0.50 | 0.0      | 3147  | SiH3+    | ELECTR  | SiH3    | H       | 1.50E-07 | -0.50 | 0.0      |
| 3156  | SiH4+    | ELECTR  | SiH3    | H       | 1.50E-07 | -0.50 | 0.0      | 3157  | SiH4+    | ELECTR  | SiH2    | H2      | 1.50E-07 | -0.50 | 0.0      |
| 3163  | SiH5+    | ELECTR  | SiH4    | H       | 1.50E-07 | -0.50 | 0.0      | 3164  | SiH5+    | ELECTR  | SiH3    | H2      | 1.50E-07 | -0.50 | 0.0      |
| 3227  | SiO+     | ELECTR  | Si       | O       | 2.00E-07 | -0.50 | 0.0      | 3247  | SiOH+    | ELECTR  | SiO     | H       | 1.50E-07 | -0.50 | 0.0      |
| 3248  | SiOH+    | ELECTR  | Si       | OH      | 1.50E-07 | -0.50 | 0.0      | 3247  | SiOH+    | ELECTR  | SiO     | H       | 1.50E-07 | -0.50 | 0.0      |
| 3247  | SiOH+    | ELECTR  | Si       | OH      | 1.50E-07 | -0.50 | 0.0      | 3247  | SiOH+    | ELECTR  | SiO     | H       | 1.50E-07 | -0.50 | 0.0      |

EROSI Mg** +He = GRAIN He Mg 1.221D-2 73.0 41.187
EROSI Fe** +He = GRAIN He Fe 1.151D-2 73.0 40.976
EROSI Si** +He = GRAIN He Si 1.224D-2 73.0 42.175
EROSI Mg** +He = GRAIN He O 5.348D-2 73.0 36.030
EROSI Si** +He = GRAIN H Mg 2.935D-2 48.0 36.740
EROSI Si** +He = GRAIN C Fe 2.386D-2 47.0 37.940
EROSI Si** +He = GRAIN C Si 2.698D-2 48.0 36.502
EROSI Si** +He = GRAIN C C 2.698D-2 48.0 36.502
EROSI Si** +He = GRAIN C O 1.054D-1 48.0 38.812
EROSI Mg** +He = GRAIN N Mg 2.935D-2 48.0 36.740
EROSI Fe** +He = GRAIN N Fe 2.386D-2 47.0 42.794
EROSI Si** +He = GRAIN N Si 2.698D-2 48.0 36.502
EROSI C** +He = GRAIN N C 2.698D-2 48.0 36.502
EROSI C** +He = GRAIN N O 1.054D-1 48.0 38.812
EROSI Mg** +He = GRAIN N Mg 2.935D-2 48.0 36.740
EROSI Fe** +He = GRAIN N Fe 2.386D-2 47.0 42.794
EROSI Si** +He = GRAIN N Si 2.698D-2 48.0 36.502
EROSI C** +He = GRAIN N C 2.698D-2 48.0 36.502
EROSI C** +He = GRAIN N O 1.054D-1 48.0 38.812
EROSI Mg** +He = GRAIN N Mg 2.935D-2 48.0 36.740
EROSI Fe** +He = GRAIN N Fe 2.386D-2 47.0 42.794
EROSI Si** +He = GRAIN N Si 2.698D-2 48.0 36.502
EROSI C** +He = GRAIN N C 2.698D-2 48.0 36.502
EROSI C** +He = GRAIN N O 1.054D-1 48.0 38.812
EROSI Mg** +He = GRAIN O Mg 2.884D-2 48.0 30.238
EROSI Fe** +He = GRAIN O Fe 4.116D-2 44.0 59.438
EROSI Si** +He = GRAIN O Si 3.373D-2 47.0 37.810
EROSI C** +He = GRAIN O C 3.373D-2 47.0 37.810
EROSI C** +He = GRAIN O O 1.006D-1 47.0 31.588
EROSI Mg** +H2O = GRAIN H2O Mg 2.884D-2 48.0 38.238
EROSI Fe** +H2O = GRAIN H2O Fe 4.116D-2 44.0 59.438
EROSI Si** +H2O = GRAIN H2O Si 3.373D-2 47.0 37.810
EROSI C** +H2O = GRAIN H2O C 3.373D-2 47.0 37.810
EROSI C** +H2O = GRAIN H2O O 1.006D-1 47.0 31.588
EROSI Mg** +N2 = GRAIN N2 Mg 2.093D-2 48.0 28.730
EROSI Fe** +N2 = GRAIN N2 Fe 4.324D-2 47.0 42.335
EROSI Si** +N2 = GRAIN N2 Si 2.217D-2 47.0 28.013
EROSI C** +N2 = GRAIN N2 C 2.217D-2 47.0 28.013
EROSI C** +N2 = GRAIN N2 O 1.149D-1 46.0 46.018
EROSI Mg** +C0 = GRAIN C0 Mg 2.093D-2 48.0 27.730
EROSI Fe** +C0 = GRAIN C0 Fe 4.324D-2 47.0 42.335
EROSI Si** +C0 = GRAIN C0 Si 2.217D-2 47.0 28.013
EROSI C** +C0 = GRAIN C0 C 2.217D-2 47.0 28.013
EROSI C** +C0 = GRAIN C0 O 1.149D-1 46.0 46.018
EROSI Mg** +02 = GRAIN O2 Mg 2.093D-2 48.0 27.730
EROSI Fe** +02 = GRAIN O2 Fe 4.324D-2 47.0 42.335
EROSI Si** +02 = GRAIN O2 Si 2.217D-2 47.0 28.013
EROSI C** +02 = GRAIN O2 C 2.217D-2 47.0 28.013
EROSI C** +02 = GRAIN O2 O 1.149D-1 46.0 46.018
ADSOR C +GRAIN = CH4* 1.00D+00 102.
ADSOR CH +GRAIN = CH4* 1.00D+00 102.
ADSOR CH2 +GRAIN = CH4* 1.00D+00 102.
ADSOR CH3 +GRAIN = CH4* 1.00D+00 102.
ADSOR CH4 +GRAIN = CH4* 1.00D+00 102.
ADSOR O +GRAIN = H2O* 1.00D+00 102.
ADSOR O2 +GRAIN = O2* 1.00D+00 102.
ADSOR OH +GRAIN = H2O* 1.00D+00 102.
ADSOR H20 +GRAIN = H2O* 1.00D+00 102.
ADSOR C0 +GRAIN = C0* 1.00D+00 102.
ADSOR C02 +GRAIN = C02* 1.00D+00 102.
ADSOR C2 +GRAIN = CH4* 1.00D+00 102.
| Reaction                      | Energy (kcal/mol) |
|-------------------------------|-----------------|
| **Adsorption**                |                 |
| ADSOR C2H + GRAIN = CH4* CH4* | 1.000±00        |
| ADSOR C2H2 + GRAIN = CH4* CH4* | 1.000±00        |
| ADSOR C3 + GRAIN = CH4* CH4* CH4* | 1.000±00        |
| ADSOR C3H + GRAIN = CH4* CH4* CH4* | 1.000±00        |
| ADSOR C3H2 + GRAIN = CH4* CH4* CH4* | 1.000±00        |
| ADSOR C3 + GRAIN = CH4* NH3* | 1.000±00        |
| ADSOR NH3 + GRAIN = NH3* | 1.000±00        |
| ADSOR NH2 + GRAIN = NH3* | 1.000±00        |
| ADSOR CN + GRAIN = CH4* NH3* | 1.000±00        |
| ADSOR HCN + GRAIN = CH4* NH3* | 1.000±00        |
| ADSOR HNC + GRAIN = CH4* NH3* | 1.000±00        |
| ADSOR N2 + GRAIN = NH3* | 1.000±00        |
| ADSOR NO + GRAIN = H2O* NH3* | 1.000±00        |
| ADSOR CH4* + HCN = CH4* NH3* | 1.000±00        |
| ADSOR HNC = CH4* NH3* | 1.000±00        |
| ADSOR N2 = CH4* NH3* | 1.000±00        |
| **Desorption**                |                 |
| DESOR CH4* + CRP = CH4 GRAIN | 7.000±01        |

| Reaction                      | Energy (kcal/mol) |
|-------------------------------|-----------------|
| SPUTT CH4* + H = CH4 H GRAIN | 4.000-05        |
| SPUTT CH4* + H2 = CH4 H2 GRAIN | 1.000-04        |
| SPUTT CH4* + He = CH4 He GRAIN | 8.000-04        |
| SPUTT O2* + H = O2 H GRAIN | 4.000-05        |
| SPUTT O2* + H2 = O2 H2 GRAIN | 1.000-04        |
| SPUTT H2O* + H = H2O H GRAIN | 4.000-05        |
| SPUTT H2O* + H2 = H2O H2 GRAIN | 1.000-04        |
| SPUTT CO* + H = CO H GRAIN | 4.000-05        |
| SPUTT CO* + H2 = CO H2 GRAIN | 1.000-04        |
| SPUTT CO2* + He = CO2 He GRAIN | 8.000-04        |
| SPUTT HCO2H* + H = HCO2H H GRAIN | 4.000-05        |
| SPUTT HCO2H* + H2 = HCO2H H2 GRAIN | 1.000-04        |
| SPUTT HCO2H* + He = HCO2H He GRAIN | 8.000-04        |
| SPUTT H2CO* + H = H2CO H GRAIN | 4.000-05        |
| SPUTT H2CO* + H2 = H2CO H2 GRAIN | 1.000-04        |
| SPUTT H2CO* + He = H2CO He GRAIN | 8.000-04        |
| SPUTT H2O2H* + H = H2O2H H GRAIN | 4.000-05        |
| SPUTT H2O2H* + H2 = H2O2H H2 GRAIN | 1.000-04        |
| SPUTT H2O2H* + He = H2O2H He GRAIN | 8.000-04        |
| SPUTT OCS* + H = OCS H GRAIN | 4.000-05        |
| SPUTT OCS* + H2 = OCS H2 GRAIN | 1.000-04        |
| SPUTT OCS* + He = OCS He GRAIN | 8.000-04        |
| SPUTT H2S* + H = H2S H GRAIN | 4.000-05        |
| SPUTT H2S* + H2 = H2S H2 GRAIN | 1.000-04        |
| SPUTT H2S* + He = H2S He GRAIN | 8.000-04        |
| Reaction | Reaction | Species | Units |
|----------|----------|---------|-------|
| DESOR H2O* | +CRP =H2O | GRAIN | 7.00D+01 0.00 0.0 |
| DESOR CO* | +CRP =CO | GRAIN | 7.00D+01 0.00 0.0 |
| DESOR CO2* | +CRP =CO2 | GRAIN | 7.00D+01 0.00 0.0 |
| DESOR NH3* | +CRP =NH3 | GRAIN | 7.00D+01 0.00 0.0 |
| DESOR CH3OH* | +CRP =CH3OH | GRAIN | 7.00D+01 0.00 0.0 |
| DESOR H2CO* | +CRP =H2CO | GRAIN | 7.00D+01 0.00 0.0 |
| DESOR HCO2H* | +CRP =HCO2H | GRAIN | 7.00D+01 0.00 0.0 |
| DESOR OCS* | +CRP =OCS | GRAIN | 7.00D+01 0.00 0.0 |
| DESOR H2S* | +CRP =H2S | GRAIN | 7.00D+01 0.00 0.0 |
| G  | +ELECTR =G- | PHOTON | 6.900D-5 0.50 0.0 |
| G-  | +H+ =G  | H  | 1.60D-06 0.50 0.0 |
| G-  | +H3+ =G  | H2  | 4.61D-07 0.50 0.0 |
| G-  | +H3+ =G  | H  | 4.61D-07 0.50 0.0 |
| G-  | +He+ =G  | He  | 8.00D-07 0.50 0.0 |
| G-  | +C+ =G  | C  | 4.61D-07 0.50 0.0 |
| G-  | +H3O+ =G  | H2O  | 3.66D-07 0.50 0.0 |
| G-  | +H3S+ =G  | H2S  | 2.70D-07 0.50 0.0 |
| G-  | +NH4+ =G  | NH3  | 3.76D-07 0.50 0.0 |
| G-  | +HCO+ =G  | CO  | 2.96D-07 0.50 0.0 |
| G-  | +HC5+ =G  | CS  | 2.38D-07 0.50 0.0 |
| G-  | +Si+ =G  | Si  | 3.01D-07 0.50 0.0 |
| G-  | +Fe+ =G  | Fe  | 2.13D-07 0.50 0.0 |
| G-  | +S+ =G  | S  | 2.82D-07 0.50 0.0 |
| G  | +H+ =G+ | H  | 1.60D-06 0.50 0.0 |
| G  | +H3+ =G+ | H2  | 4.61D-07 0.50 0.0 |
| G  | +H3+ =G+ | H  | 4.61D-07 0.50 0.0 |
| G  | +He+ =G+ | He  | 8.00D-07 0.50 0.0 |
| G  | +C+ =G+ | C  | 4.61D-07 0.50 0.0 |
| G  | +H3O+ =G+ | H2O  | 3.66D-07 0.50 0.0 |
| G  | +H3S+ =G+ | H2S  | 2.70D-07 0.50 0.0 |
| G  | +NH4+ =G+ | NH3  | 3.76D-07 0.50 0.0 |
| G  | +HCO+ =G+ | CO  | 2.96D-07 0.50 0.0 |
| G  | +HC5+ =G+ | CS  | 2.38D-07 0.50 0.0 |
| G  | +Si+ =G+ | Si  | 3.01D-07 0.50 0.0 |
| G  | +Fe+ =G+ | Fe  | 2.13D-07 0.50 0.0 |
| G  | +S+ =G+ | S  | 2.82D-07 0.50 0.0 |
| G+ | +ELECTR =G  | PHOTON | 6.900D-5 0.50 0.0 |
| G  | +SECPHO =G+ | ELECTR | 0.63D+08 0.00 140000.0 |
| G- | +SECPHO =G  | ELECTR | 0.41D+09 0.00 140000.0 |

END

Table H.1: Full chemical network for the Paris-Durham shock code.
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Abstract

Stars are bad neighbors: they often disturb their surroundings. They sometimes travel very fast through the interstellar medium (ISM). They frequently undergo violent ejection events which leave an imprint on their neighborhood (jets, winds, supernovae). These supersonic flows generate shocks both in the ejected material (bow shock) and in the stellar environment (termination shock). The global purpose of this thesis is to link the properties of stars and the ISM by studying these shocks. We model them with the Paris-Durham planar shock code, which incorporates a wealth of micro-physics and chemical processes relevant to the magnetized ISM.

In the first part, we model 3D magnetized axisymmetric bow shock by a statistical distribution of 1D planar shocks computed with the Paris-Durham model. For the first time, we examine systematically the effect of the geometry, age, and various other parameters on the H$_2$ excitation diagram and emission line profiles. Then, we will show that this 3D bow shock model unprecedentedly improves interpretations of the H$_2$ observations in Orion BN-KL and BHR71, and show how spectrally resolved H$_2$ line emission profiles on the Herbig-Haro object HH54 can be used to extract a wealth of dynamical information.

In the second part, we model 1D steady stellar winds from AGB stars, which trigger the termination shock, by including relevant physical and chemical ingredients in the Paris-Durham code. For the first time, we examine the time-dependent conversion of atomic to molecular hydrogen along the wind trajectories of “hot” and “cold” AGB stars. We suggest that the low abundance of HI inferred from observations is due to hydrogen locked in its molecular form. Then, we try to reproduce HI 21-cm line profile in a “hot” AGB (called Y Cvn) and a “cold” AGB (called CW Leo).

Keywords
Shock waves – Herbig-Haro objects – ISM: jets and outflows – ISM: molecules
Stars: abundances – Stars: AGB and post-AGB – Stars: Winds, outflows