

AGB outflows as tests of chemical kinetics and radiative transfer models

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Abstract. The outflows of asymptotic giant branch (AGB) stars are important astrochemical laboratories, rich in molecular material and host to various chemical processes, including dust formation. Since the different chemistries are relatively easily probed, AGB outflows are ideal testbeds within the wider astrochemical community. Recent observations are pushing the limits of both our current chemical models and radiative transfer routines. Current chemical models are restricted by the completeness of their chemical networks and the accuracy of the reaction rates. The molecular abundances retrieved by radiative transfer routines are strongly dependent on collisional rates, which are often not measured or calculated for molecules of interest. To further our understanding of the chemistry within the outflow, collaboration with the laboratory astrophysics community is essential. This collaboration is mutually beneficial, as it in turn provides new science questions for laboratory experiments and computations.

Keywords. astrochemistry, molecular processes, stars: AGB and post-AGB stars, circumstellar material, stars: mass loss

1. Introduction

During the asymptotic giant branch (AGB) phase, low-to-intermediate mass stars lose their outer layers by means of a stellar outflow, creating an extended circumstellar envelope (CSE). These CSEs are rich astrochemical laboratories, with close to 100 molecules as well as dust particles detected therein. They are typically divided into two chemical groups: the oxygen-rich and the carbon-rich CSEs. Thanks to the wide ranges in temperature and density throughout the CSE, they host a varied chemistry. In the inner CSE, close to the star, shocks caused by the pulsating AGB star take the chemistry out of thermodynamic equilibrium. Further out, in the intermediate wind, solid-state dust grains condense from the gas phase, launching the dust-driven wind that determines the final fate of the star and creates the CSE. Finally, in the outer wind, the chemistry is mainly photon-driven due to the lower density within this region.

Chemistry and dynamics are coupled throughout the outflow. A better understanding of the chemistry therefore leads to a greater knowledge of the dynamics, and by extension stellar evolution and the enrichment of the interstellar medium (ISM) with both gas and dust. The critical process of dust formation remains elusive, especially for oxygen-rich CSEs, for which we still do not know how the first seed particles are formed and how these grow to larger dust grains. Thanks to the various chemical processes within the outflow and its relatively simple dynamical structure, CSEs are moreover valuable chemical laboratories to the entire laboratory astrophysics community.

Recent observations are pushing the limits of our modelling efforts. Our current chemical models, necessary to deduce the specific chemical pathways throughout the outflow,

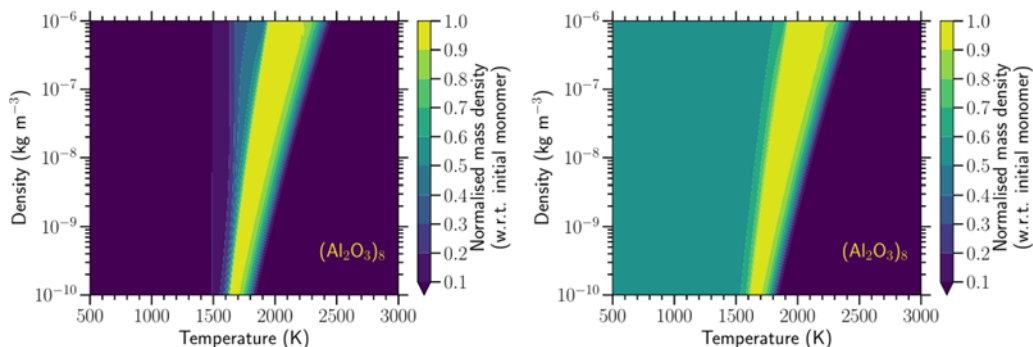


Figure 1. Normalised mass density (or mass fraction) with respect to the initially available Al_2O_3 monomer abundance. Left: results using the monomer nucleation description. Right: results using the polymer nucleation description. From [Boulangier *et al.* \(2019\)](#).

and our radiative transfer routines, crucial to retrieve accurate abundances of both the gas-phase and dusty components, are limited by the available laboratory data. We highlight some of the current issues.

2. Dust formation

Dust formation is relatively well-understood in carbon-rich CSEs, where small carbon-bearing molecules cluster together, forming larger sooty particles and PAHs (e.g. [Frenklach & Feigelson 1989](#); [Cherchneff *et al.* 1992](#)).

For oxygen-rich CSEs, however, the seed particles and nucleation pathways are still not known. Recent SPHERE observations of the inner wind of the oxygen-rich AGB star R Dor revealed that dust is present close to its stellar surface ([Khouri *et al.* 2016](#)). Several candidates for the dust composition exist. Through radiative transfer modelling, [Decin *et al.* \(2017\)](#) have shown that the majority of Al is not locked up in molecules, which points towards the presence of Al_2O_3 dust. However, state-of-the-art forward modelling of the inner CSE, coupling hydrodynamics and chemistry, can only produce Al_2O_3 clusters if the monomer is present. When starting the model with a purely atomic composition, most of the Al remains atomic ([Boulangier *et al.* 2019](#)). This points to either inaccurate reaction rates involving the formation of the monomer, missing Al_2O_3 cluster formation pathways, or both. [Boulangier *et al.* \(2019\)](#) also show that allowing nucleation through polymer interaction, and not only monomer interactions as is classically assumed, yields a larger abundance of clusters close to the star (Fig. 1).

3. Chemical and radiative transfer modelling of the gas phase

The abundances of gas-phase species throughout the outflow are retrieved from observations using radiative transfer modelling. To do so, collisional excitation rates of the molecules of interest need to be known.

3.1. Oxygen-rich CSEs

[Danilovich *et al.* \(2017\)](#) have demonstrated the importance of these collisional rates when retrieving the H_2S abundance within a sample of CSEs. Two sets of collisional rates exist for H_2S . Neither of them are based on H_2S specific calculations or measurements, as both are obtained from scaling H_2O collisional rates. The LAMBDA rates ([Schöier *et al.* 2005](#)) are based on those determined by [Dubernet *et al.* \(2006, 2009\)](#) and [Daniel *et al.* \(2010, 2011\)](#). The JHB rates include those measured by [Faure *et al.* \(2007\)](#). When

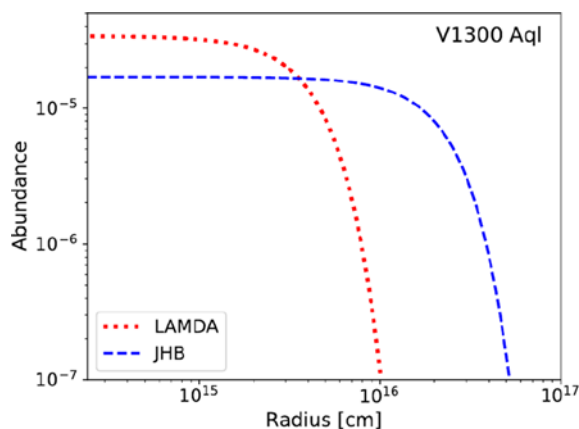


Figure 2. An example of the different H₂S abundance profiles, derived from the same observations using the two different sets of collisional rates. Image reproduced with permission from Danilovich *et al.* (2018), copyright by Galaxies.

modelling the same data, the different sets yield very different abundance profiles (Fig. 2). van der Tak (2011) suggests to use the rates of Dubernet *et al.* (2006) for cold temperatures (< 20 K), those of Faure *et al.* (2007) for warm temperatures (~ 300 K), and another set by Faure & Josselin (2008) for hot temperatures (> 300 K). However, these temperature regimes are all present throughout the CSE. Additionally, by simply scaling the H₂O collisional rates, differences in molecular cross section and dipole moments are not taken into account Danilovich *et al.* (2017).

3.2. Carbon-rich CSEs

IRC+10216 is the most studied carbon-rich AGB star. Its outflow is not smooth: density-enhanced shells are visible throughout the outflow. These shells are moreover distinctly clumpy (Agúndez *et al.* 2017). Despite several studies, the relative distribution of the cyanopolyynes, HC_{2n+1}N, and hydrocarbon radicals, C_nH ($n = 1, 2, 3, \dots$), within its CSE is not yet understood. They are located in molecular shells surrounding the star, as expected from a bottom-up formation scenario of UV-driven synthesis. In this scenario, the molecules are distributed following a radial sequence of increasingly complex molecules. The cyanopolyynes follow such a radial distribution (Millar & Herbst 1994; Millar *et al.* 2000; Agúndez *et al.* 2017). The hydrocarbon radicals, however, are observed to be cospatial (Guélin *et al.* 1993, 1999; Agúndez *et al.* 2017). Several chemical models have attempted to explain this behaviour. They have taken into account either the density-enhanced shells (Cordiner & Millar 2009) or the increased UV radiation throughout the CSE due to the clumpiness of the shells (Agúndez *et al.* 2017). Both approaches result in a cospatial behaviour of the hydrocarbon radicals as well as the cyanopolyynes. Using the chemical model of Van de Sande *et al.* (2018), which simultaneously takes into account density-enhancements and an increased UV radiation field, we attempt to determine their relative importance. However, in order to compare our calculated abundance profiles to the observations, radiative transfer modelling with accurate collisional rates is needed. Since collisional rates are only available for HC₃N, we have to resort to scaling laws, which do not take into account differences in molecular cross section and dipole moments, severely restricting our modelling efforts (Van de Sande *et al.* in prep).

4. Conclusions

Understanding the rich chemistry inside AGB outflows is not only of interest to the AGB community, as it provides a greater insight in its dynamics, but to the wider laboratory astrophysics community. The different types of chemistry, including dust formation, can be easily probed thanks to the comparatively simple dynamical structure of the outflow, making CSEs an ideal testbed for these various processes. To extract scientific insights from observations, chemical models and radiative transfer routines are used. Recent advances in observations have, however, reached the current limits of our models. Future observations, in particular the ALMA Large Program ATOMIUM (PI L. Decin), are certain to require even more modelling efforts. In order to fully exploit the wealth of observational data, laboratory data are imperative.

Chemical models require accurate chemical reaction rates and complete chemical networks. This is not only important for the elusive dust formation mechanism in oxygen-rich AGB outflows, but also for the gas-phase chemistry in both carbon- and oxygen-rich outflows. Accurately retrieving molecular abundances throughout the outflow using radiative transfer routines depends on the collisional rates used. Not all molecules have measured collisional rates, which strongly influences the retrieved abundances. The lack of collisional rates also inhibits the comparison between the forward chemical models and the retrieved abundance profiles. A mutually beneficial collaboration between the AGB and laboratory astrophysics communities is hence imperative to better understand the chemistry within CSEs. While laboratory astrophysics will provide crucial data for our models, the AGB community will in turn produce new science questions for laboratory experiments and computations.

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