Astrochemistry VII – Through the Cosmos
from Galaxies to Planets
Proceedings IAU Symposium No. 332, 2017
M. Cunningham, T. Millar & Y. Aikawa, eds.

doi:10.1017/S1743921317007724

Determining the effect of a non-uniform AGB outflow on its chemistry

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Abstract. The molecular composition of the stellar outflows of AGB stars is determined by the stellar elemental carbon-to-oxygen abundance ratio, together with the physical circumstances in the innermost region of the outflow. Near the stellar surface, thermal equilibrium (TE) can be assumed. This leads to a certain molecular composition with a O- or C-rich signature. However, several molecular species have been detected that are not expected to be present in the inner region under the assumption of TE chemistry. As a solution to explain the presence of these unexpected species, non-equilibrium chemistry in the inner region of the outflow has been proposed. The outflows of AGB stars are generally not spherically symmetric or homogeneous, which influences the penetration of interstellar UV photons throughout the outflow. We investigate the effect of a clumpy, non-homogeneous outflow on the composition of the inner region by introducing a simple porosity formalism in our chemical model.

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

1. Introduction

The final life stage of low- to intermediate-mass stars, the asymptotic giant branch (AGB) phase, is characterised by strong mass loss via a stellar outflow. This outflow removes the outer layers of the star and creates a large circumstellar envelope. The elemental carbon-to-oxygen abundance ratio of the central AGB star determines the molecular composition of the outflow, together with the physical conditions in its innermost region. Thermal equilibrium (TE) can be assumed at the stellar surface, leading to a certain molecular composition with a O- or C-rich nature. However, several molecular species have been detected that are not expected to be present in the inner region under the assumption of TE chemistry, such as the C-rich CO_2, HCN, CS, and CN in the outflows of O-rich stars (Omont *et al.* (1993), Bujarrabal *et al.* (1994), Justtanont *et al.* (1996)) and warm H_2O for a C-rich outflow (Decin *et al.* (2010)). NH_3 has been observed with abundances higher than predicted by TE chemistry in both O- and C-rich stars (Keady *et al.* (1993), Menten *et al.* (1995)). As a solution to the presence of these unexpected species, pulsation-induced non-equilibrium chemistry in the inner region of the outflow has been proposed (Duari *et al.* (1999), Cherchneff (2006), Gobrecht *et al.* (2016)). These models are able to account for the abundances of most unexpected species, but are unable to account for e.g. NH_3 in O-rich stars (Gobrecht *et al.* (2016)).

The outflows of AGB stars are generally not spherically symmetric. Both large-scale structures, such as spirals (e.g. Maercker *et al.* (2012)) and disks (e.g. Kervella *et al.* (2014)), and small-scale density inhomogeneities (e.g. Khouri *et al.* (2016), Agúndez *et al.* (2017)) have been observed. We investigate the potential effects of small-scale density

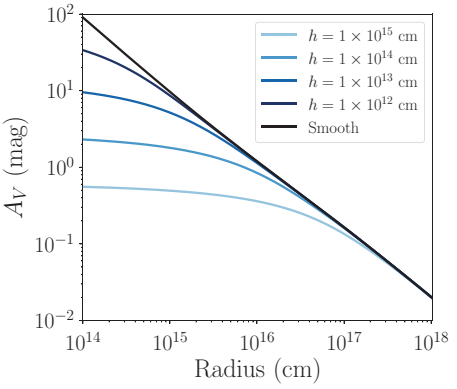

Figure 1. Visual extinction throughout a clumpy outflow with mass-loss rate 10^{-5} $M_\odot$ yr^{-1} where all material is located inside of clumps (void inter-clump component). Result for a smooth outflow is shown in black. Results for different values of the porosity length h are shown in blue.

inhomogeneities or clumps within the outflow on the composition of the inner region. This is done by introducing a porosity formalism in our chemical model.

2. Methods

2.1. *Chemical model*

The chemical reaction network used in our chemical model is the most recent release of the UMIST Database for Astrochemistry (UDfA), RATE12 (McElroy *et al.* (2013)), a gas-phase only network. The chemical model itself is based on the UDfA CSE model. This is a one-dimensional model describing a uniformly expanding, spherically symmetric outflow with a constant mass-loss rate. The physical parameters and parent species of the model are taken from Agúndez *et al.* (2010). We have modified the temperature profile of the code to a power-law, and have implemented the porosity formalism (see Sect. 2.2).

2.2. *Porosity formalism*

The porosity formalism used in this work (Owocki *et al.* (2004), Owocki *et al.* (2006), Sundqvist *et al.* (2012), Sundqvist *et al.* (2014)) provides us with a mathematical framework that describes the resultant effect of a stochastic distribution of clumps in an outflow on the intensity of the external radiation field throughout the outflow. This description is included in the code by changing the optical depth τ of a smooth outflow to the effective optical depth $\tau_{\rm eff}$ of a clumpy one, which then accounts for potential light-leakage through porous channels within the clumpy outflow. Our porosity formalism also divides the outflow into two separate components: an overdense clump component and a rarefied inter-clump component. The division between the two components is determined via the volume filling factor $f_{\rm vol}$, which is the fraction of the total volume of the outflow occupied by clumps, and the density contrast $f_{\rm ic}$, which establishes the density of the inter-clump component relative to the spatially averaged density of the outflow. A void inter-clump component corresponds to $f_{\rm ic} = 0$.

Porosity affects the visual extinction throughout the outflow. This is shown in Fig. 1 for an outflow where all material is located inside of clumps (void inter-clump medium). The porosity length h represents the local mean free path between two clumps. Using the formalism, we can hence take both the larger density of the clumps and the decrease in visual extinction throughout the outflow into account.

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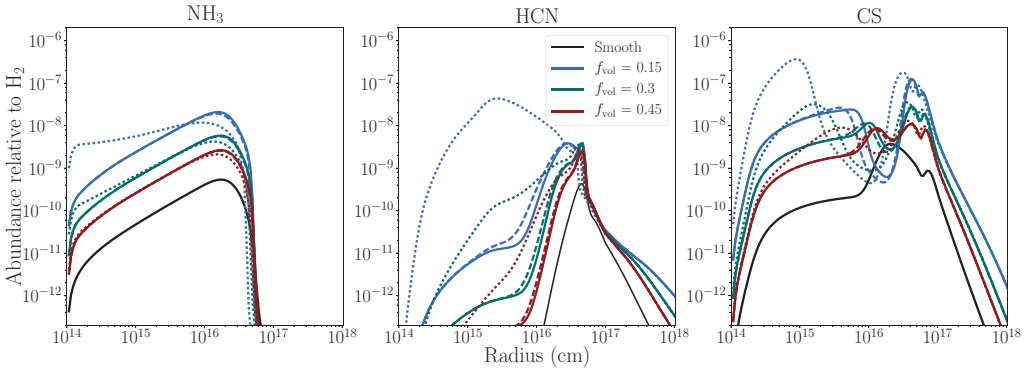

Figure 2. Abundance of NH_3, HCN, and CS relative to H_2 throughout a one-component O-rich outflow with a mass-loss rate of 10^{-5} $M_\odot$ yr^{-1} for different clump volume filling factors f_{vol}. Solid black line: calculated abundance for a smooth, uniform outflow. Solid coloured line: $l_* = 5\times10^{12}$ cm. Dashed coloured line: $l_* = 1 \times 10^{13}$ cm. Dotted coloured line: $l_* = 5 \times 10^{13}$ cm.

Table 1. Column density of NH_3, HCN, and CS in a smooth O-rich outflow with a mass-loss rate of 10^{-5} $M_\odot$ yr^{-1}, together with column density ratios relative to the smooth outflow for specific one-component outflows. The corresponding abundance profiles are shown in Fig. 2.

Species	NH_3			HCN			CS		
Smooth outflow	1.8e+12			4.2e+10			4.2e+12		
f_{vol}	0.15	0.30	0.45	0.15	0.30	0.45	0.15	0.30	0.45
$l_* = 5 \times 10^{12}$ cm	3.3e+02	4.2e+01	1.2e+01	2.1e+02	3.6e+01	1.3e+01	5.3e+02	6.2e+01	1.7e+01
$l_* = 1 \times 10^{13}$ cm	3.2e+02	4.2e+01	1.2e+01	2.4e+02	3.9e+01	1.3e+01	5.3e+02	6.2e+01	1.7e+01
$l_* = 5 \times 10^{13}$ cm	1.2e+03	4.9e+01	1.2e+01	4.5e+04	1.4e+02	2.3e+01	8.4e+03	2.7e+02	3.5e+01

3. Effect on chemistry

In Fig. 2, we show the effect of clumpiness on the abundance profiles of NH_3, HCN, and CS in an O-rich outflow with a mass-loss rate of 10^{-5} $M_\odot$ yr^{-1}. All material of the outflow is located inside of clumps, the inter-clump medium is void ($f_{ic} = 0$). The central star has a radius of 5×10^{13} cm. Our model is calculated from 2 R_* onwards.

It is clear that both the overdensity of the clumps and the porosity-associated decrease in visual extinction have an effect on the chemistry. For smaller values of f_{vol}, the overdensity of the clumps is larger, resulting in an overall larger abundance of the species. For larger values of h, more interstellar UV photons are able to reach the inner wind and release the deficient element through photodissociation. This results in the production of HCN and NH_3 closer to the central star. Using the porosity formalism, we are therefore able to produce both HCN and NH_3 in the inner region of the outflow.

A clumpy outflow not only influences the abundances in the inner region, but also affects the chemistry throughout the outflow. This can be seen in the abundance profile of CS: clumpiness of the outflow clearly alters its formation and destruction pathways in the intermediate wind, resulting in a different shape of the abundance profile.

The change in column density relative to a smooth outflow is given in Table 1. We find that the column density increases with decreasing f_{vol} for all three species. The relative increase in column density is larger for smaller values of f_{vol}: for $f_{vol} = 0.15$, the column density can be up to two orders of magnitude larger relative to a smooth outflow. The size of the clumps l_*, and therefore the porosity length h, affects the column density only when the UV field throughout the outflow is large enough to influence the chemistry and

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increase the abundance in the inner region. In that case, the column density increases by an order of magnitude relative to a smooth outflow for the same value of $f_{\rm vol}$.

In a forthcoming paper, we will additionally describe the effect of a clumpy outflow on its chemistry for a two-component medium and for several mass-loss rates, and this for both an O- and C-rich chemistry.

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