

Dynamics, temperature, chemistry, and dust: Ingredients for a self-consistent AGB wind

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Abstract. Understanding Asymptotic Giant Branch (AGB) stars is important as they play a vital role in the chemical life cycle of galaxies. AGB stars are in a phase of their life time where they have almost ran out of fuel and are losing vast amounts of material to their surroundings, via stellar winds. As this is an evolutionary phase of low mass stars, almost all stars go through this phase making them one of the main contributors to the chemical enrichment of galaxies. It is therefore important to understand what kind of material is being lost by these stars, and how much and how fast. This work summarises the steps we have taken towards developing a self-consistent AGB wind model. We improve on current models by firstly coupling chemical and hydrodynamical evolution, and secondly by upgrading the nucleation theory framework to investigate the creation of TiO₂, SiO, MgO, and Al₂O₃ clusters.

Keywords. stars: AGB and post-AGB – stars: winds, outflows – hydrodynamics – astrochemistry – methods: numerical

1. Introduction

Detailed understanding of how AGB stars lose their material via stellar winds is hindered by insufficient high resolution observations, simplified models, and a lack of laboratory data. Ample work is being done to improve on all three limitations. This work focuses on the second, improving AGB wind models. The general hypothesis is that the mass loss mechanism of AGB stars is a combination of stellar pulsations and radiative pressure on dust grains. It is slightly more complicated as their interaction encompasses several physical and chemical processes (Fig. 1). Pulsations of the star quickly turn into shock waves, as their velocities exceed the local sound speed, hereby heating up the gas. This influence on temperature affects the chemical composition of the gas, because chemical reactions behave differently at high and low temperatures. In turn, the chemical composition regulates the temperature of the gas, because the efficiency of different heating and cooling mechanisms is determined by the abundance of heating and cooling species. Meanwhile, photons from the star interact with dust grains, transferring their momentum either via absorption or scattering, hereby pushing the grains outwards. The outward moving dust then collides with the nearby gas, dragging it along towards the interstellar medium. Both driving forces, pulsations and radiation on dust grains, have been studied extensively. Yet, the link between them has mainly been ignored. Since the stellar surface does not contain any dust grains, a phase transition from gaseous material to solid grains has to occur. Due to the low density in an AGB wind, this does not happen instantly (as compared to Earth/lab conditions). On a microscopic level, the initiation of a phase transition is called nucleation. This process corresponds to molecules reacting with each other to form larger clusters, either homomolecular (same species) or

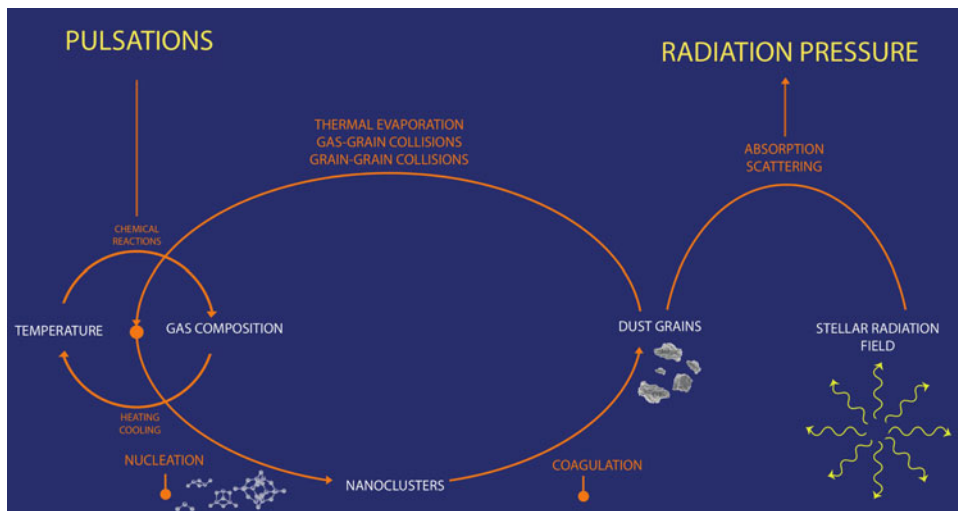


Figure 1. Schematic, yet simplified, overview of the physical and chemical processes occurring in an AGB wind. The two main driving forces are pulsations of the star and radiation pressure on dust grains. Both are self-consistently connected via the mechanisms depicted in the figure.

heteromolecular (different species). From a certain size, physical forces will take over, e.g. van der Waals, and such nanoclusters will coagulate to form macroscopic dust grains. In turn, dust grains can be destroyed by thermal evaporation, gas-grain collisions, and grain-grain collisions, hereby shattering the grains and/or liberating gaseous material. The combination of dynamical and chemical evolution (hydrochemistry), interaction of dust grains with stellar radiation, and the missing link of dust evolution with creation from gas, makes a self-consistent AGB wind model. Such a model will aid in understanding what kind of material is being lost by these stars, and how much and how fast.

2. Hydrochemistry

Driving an AGB wind purely hydrodynamically is unfeasible when using a physically reasonable pulsation behaviour. The gravitational pull of the star is too large for the gas to exceed the local escape velocity. It is however possible to hydrodynamically drive the wind when increasing the pulsational velocity variation at the stellar surface by roughly an order of magnitude. Yet, this is most likely unrealistic. As suggested by the current hypothesis, extra outward force by radiation pressure on dust grain can aid in driving the wind. Because dust formation is highly sensitive to temperature, which also depends on the chemical composition, one has to precisely know the gas composition and its temperature. This can only be achieved by a hydrochemical simulation, since the chemical composition and temperature mutually affect one another, by temperature dependency of chemical reactions and by abundances of heating and cooling species. However, current AGB wind models have ignored this and assume chemical equilibrium (e.g. Bowen 1988, Willson 2000, Woitke 2006, Höfner *et al.* 2016). We improve on these models by introducing non-equilibrium chemical evolution (also done in static AGB wind models, Cherchneff 2012, Marigo *et al.* 2016, Gobrecht *et al.* 2016) and couple this to the dynamics of the wind, called hydrochemistry (Boulanger *et al.* 2018).

We have constructed a chemical reaction network which is applicable to AGB winds, yet still simplified. The bulk of the reactions originates from the UMIST database, extended with a handful from the KIDA database and standalone papers. In total, the network comprises roughly 1700 reactions and 160 species. This has to be reduced when coupled to a hydrodynamical framework, due to computational constraints. After applying a

reduction algorithm to identify the most important reactions, we end up with roughly 250 reactions and 70 species, resulting in a speedup factor of 20. The algorithm makes sure that the non-reduced results are reproduced within a certain accuracy, for an AGB wind environment.

We have modelled a 1D AGB wind using the hydrodynamics code MPI-AMRVAC (Keppens *et al.* 2012) and chemistry code KROME (Grassi *et al.* 2014). The former had to be extended to be able to handle conservation of chemical species (Plewa & Müller 1999) and have a variable adiabatic index that depends on the local chemical composition.

3. Nucleation theory

Current AGB wind models assume some dust growth mechanism starting from the artificial presence of dust seed particles (typically molecules consisting of 100 – 1000 of monomers), e.g., Höfner *et al.* 2016. Such seed particles actually have to form by nucleation of gas molecules. Several prescriptions have been used in closed systems in the literature: classical, modified, and kinetic steady state nucleation theory (Helling & Woitke 2006, Gail *et al.* 2013, Köhler *et al.* 1997, Patzer *et al.* 1998, Bromley *et al.* 2016, Goumans *et al.* 2012, Plane 2013). Also outside of AGB modelling, e.g. brown dwarf atmospheres (Lee *et al.* 2018), and supernovae (Nozawa & Kozasa 2013, Lazzati & Heger 2016). We perform a two-step improvement on such models, firstly with non-equilibrium time-dependent nucleation, and secondly coupling this to a large chemical network (Boulangier *et al.* in prep.); its closest resemblance is the “molecular nucleation theory” of Sluder *et al.* (2018)). Our first improvement “non-equilibrium time-dependent nucleation” corresponds to clusters growth reactions by monomer addition and destruction reactions based on the assumption of detailed balance. This latter uses the Gibbs free energy of the clusters, which are calculated from first principles. Density functional theory is used to determine electronic structures, rotational, and vibrational degrees of freedom, all of which are needed to infer the Gibbs free energy of the molecules. This part has also been done in the past (Goumans *et al.* 2012, Lee *et al.* 2018, Köhler *et al.* 1997). However, these papers assume steady state nucleation, meaning in chemical equilibrium, whereas we treat each growth/destruction reaction separately, meaning time-dependent non-equilibrium evolution. Our second improvement step is applying this nucleation theory to a chemical reaction network, starting from an atomic composition rather than the nucleating monomer. This removes the assumption of the monomer being (abundantly) present, and species can compete for chemical resources.

We consider four nucleation candidates that have been proposed in the literature: TiO₂, SiO, MgO, and Al₂O₃. The largest clusters considered consist of roughly 30 atoms. This limit is either due to lack of data/computational constraints on larger clusters or where the nucleation-by-monomer principle breaks down. Gibbs free energies of all clusters are calculated by determining the quantum chemical properties via density functional theory where we started from minimum energy configurations found in the literature. Additionally, we have searched the literature thoroughly for chemical reactions of Ti-, Mg-, Si-, and Al-bearing species to, among other, bridge the gap from atoms to nucleation monomers. We first perform ‘pure nucleation’ models for each candidate, where such a model consists of starting with a monomer abundance and evolving a system of only nucleation growth and destruction reactions over a certain period of time. After performing a grid of ‘pure nucleation’ models from 500 to 3000 K and 10⁻⁶ to 10⁻¹⁰ kg m⁻³ for one year time, we find that each candidate has a different temperature cut-off above which the largest clusters do not form. For Al₂O₃ this is around 1800 to 2200 K, for MgO around 1500 to 1700 K, for TiO₂ around 1200 to 1300 K, and for SiO around 500 K. According to these models, Al₂O₃ is the best candidate to form dust because it is desirable to form dust as fast as possible while the gas is cooling down, so as quickly as possible have an extra outwards force by radiation pressure. However, the results

differ when performing a grid of models with our second improvement, starting from an atomic composition and nucleation included in a large chemical network. Here, the Al_2O_3 monomer does not form at all, meaning none of its bigger clusters form either. MgO clusters have the same problem, namely, all Mg stays atomic, so no MgO monomers, meaning no larger clusters either. SiO clusters are equally inefficient as in the previous model, and are not of interest due to its low temperature cut-off. However, TiO_2 monomers form easily and so do their larger clusters. The abundance of TiO_2 clusters is the same as in the previous model. Thus, according to these models, TiO_2 is the favourable dust precursor. Yet, one has to be careful with drawing conclusions from these models. It is not because the models cannot produce Al_2O_3 clusters, that they don't exist in AGB winds. It does mean that with the current model we cannot form them. As Al_2O_3 clusters are abundantly present in presolar grains, originating from AGB winds, the model is most likely incomplete. It is most probably missing chemical pathways to form such clusters, others than starting from the Al_2O_3 monomer which is chemically unstable due to its triplet ground state. Our current models predict most Al stays atomic ($\sim 99\%$) and the most abundant Al-bearing molecules are AlO , AlH , AlC , AlOH , $\text{Al}(\text{OH})_2$, and $\text{Al}(\text{OH})_3$. These molecules are then good starting points for determining/calculating different reactions to form Al_2O_3 clusters, skipping its monomer.

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Discussion

QUESTION: Do you update the chemical reaction network during your hydrochemical model?

BOULANGIER: No, we determine a reduced network prior to the hydrochemical network that is valid for the parameter space of the AGB wind model (temperature, density, time).

QUESTION: Do you include ions in your calculations and what role do they play?

BOULANGIER: Yes. They play an important role in cooling the gas at high temperatures. Their importance for the composition is not immediately clear, and we have not investigated this.

QUESTION: How much confidence do you have that the TiO clusters are most relevant, given that the models reveal difficulties producing the same of the more elementary molecules?

BOULANGIER: We do not claim that TiO clusters are the most relevant. Our current models can however only produce TiO clusters efficiently. However, we mainly think that this is due to the lack of formation pathways of the other cluster candidates. For example, we find more Al_2O_3 than TiO clusters in pre-solar grains, yet we cannot produce it with the models suggesting that our model is not comprehensive enough. A possibility might be to form a larger Al_2O_3 cluster not via its monomer but by a different chemical reaction, skipping the unstable and difficult to form monomer.

QUESTION: Do you rule out that formation of alumina dust can occur, at least partly, on Al-bearing seed grains?

BOULANGIER: We do not rule this out because we do not take this into account. It might be that there is an efficient alumina dust formation pathway that is not the nucleation by monomer addition which we are currently only considering. The only way of knowing is adding more and more formation pathways and then see which ones are most efficient.

