Molecular layers in the dust formation zone of AGB stars

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Seminar
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Overview

• AGB stars: types & evolution
• The inner wind of AGB stars
• Stationary wind vs. Dynamic pulsations
• Chemical model for the gas phase, cluster formation routes and dust grains
• Results on molecules & dust clusters
• Dust condensation & grain size distributions
• Outlook & Conclusions
AGB stars

Late stage evolution of low- and intermediate stars ($M^{\text{ZAMS}} < 8 \, M_\odot$)

Cool photospheres ($T = 2000 - 3000 \, \text{K}$) and high luminosities ($L \sim 10^3 - 10^4 \, L_\odot$)

High mass loss rates ($10^{-7} - 10^{-4} \, M_\odot/\text{yr}$) due to the presence of dust
Evidence for dust

Spectral dust features (Silicates & SiC):

- Forsterite ($\text{Mg}_2\text{SiO}_4$) in the lab (69 μm):
  - Bowey 2013

- Other features:
  - MgS at 30 μm
  - PolyAromatic Hydrocarbons (PAHs) at 3.3, 6.2, 7.7, 8.8, 12.7 and 16.4 μm → (hydrogenated) amorphous carbon
**Chemical types of AGB stars**

M-type: oxygen-rich, $C/O < 1$

S-type: $C/O \sim 1$

C-type: carbon-rich, $C/O > 1$

... at the photosphere

Low mass: $3^{rd}$ dredge up mixes carbon to the photosphere $\rightarrow C/O$ increases

Intermediate mass: Hot bottom burning converts C in N and other CNO products $\rightarrow C/O$ decreases

Hoefner 2009
Thermodynamic equilibrium (TE) predicts the presence of:

- CO, C, HCN, CS, $\text{C}_2\text{H}_2$, CH, CN in the C-rich case
- CO, H$_2$O, SiO, OH, TiO in the O-rich case

$\rightarrow E_{\text{bind}}(\text{CO}) = 11.2$ eV $\rightarrow$ locks up lesser abundant element

**BUT** observed are also:

- C-bearing molecules in O-rich AGBs: HCN, CS, OCS, CN, CO$_2$
- O-bearing species in carbon stars: H$_2$O, OH, SiO

TE cannot account for these observed molecules

$\Rightarrow$ Kinetic description is necessary for the chemistry
AGB star structure

Stellar wind driven by pulsations and dust grains

Large convective envelope

Energy generation proceeds in thin burning shells

Degenerate (non-burning) core consisting of carbon and oxygen

Lattanzio 2004
The inner wind of AGBs

IK Tau

AGB star

Radius

Pulsating Photosphere

T = 2200 K
N = 10^{14} cm^{-3}

Inner envelope
Dust formation

500-42'000 K
10^{6} - 10^{16} cm^{-3}

Fully accelerated wind

100 K
10^{6} cm^{-3}

decin 2010

Interstellar
UV radiation

CO, H_{2}O
SiO

HCN, CS, CO_{2}
SiS, PN, AIOH

NH_{3}, SO_{2}
H_{2}S
daughter species produced by photo reactions of mother species
Energy scale in the wind
Timescales for AGB stars

Main sequence: \(~ 10^7 - 10^{10} \) years

Time on the (TP) AGB: \(~ 10^6 \) years

Time between dredge-up (mixing) episodes: \(~ 10^4 \) years

Maercker 2009

Timescale in the wind:
- Expansion timescale: \( \frac{R_{\text{env}}}{V_{\text{exp}}} \) ~
- Time between pulsations: \(~ 1 \) year
- Chemical reactions: \( \frac{1}{k} \) ~ ms to hours
- Dust growth: coagulation & surface growth
Physics of the inner wind

Periodic shocks cross the stellar atmosphere

→ ambient gas is compressed, heated and accelerated

→ formation of dense and warm gas layers gravitationally bound to the star

→ favourable conditions for molecule, cluster & dust grain formation


→ Pulsations & dust are necessary for mass loss

Nowotny 2010
Periodic pulsation model for a galactic Mira star: IK Tau

Pre-shock profiles:

\[ T(r) = T_\ast \left( \frac{r}{R_\ast} \right)^{-0.6} \quad n(r) \propto n_\ast \exp \left( -\frac{r}{H} \right) \]

Scale height

\[ H = \frac{k_B T}{\mu m_H g} = \frac{k_B T R^2}{\mu m_H GM} \]

Willson & Bowen 1984, Cherchneff 1992

Post-shock profiles:
- Rankine-Hugoniot jump conditions
- Gas excursions on ballistic trajectories

Based on mass,

\[ \frac{d\rho}{dt} = \left( \frac{\partial}{\partial t} + v \frac{\partial}{\partial z} \right) \rho = -\rho (\nabla \cdot v) \]

momentum, and

\[ \frac{dv}{dt} + \frac{1}{\rho} \frac{\partial p}{\partial z} = -g \]

energy

\[ \frac{dp}{dt} + \gamma \rho (\nabla \cdot v) = 0 \]

Parameters for IK Tau

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>( T_\ast )</td>
<td>2200 K</td>
</tr>
<tr>
<td>( M_\ast )</td>
<td>1 ( M_\odot )</td>
</tr>
<tr>
<td>( R_\ast )</td>
<td>2.5 ( \times 10^{13} ) cm</td>
</tr>
<tr>
<td>( \nu_s )</td>
<td>25 – 32 ( \text{km s}^{-1} )</td>
</tr>
<tr>
<td>( P )</td>
<td>470 days</td>
</tr>
<tr>
<td>( n(1R_\ast) )</td>
<td>3.6 ( \times 10^{14} ) cm(^{-3} )</td>
</tr>
<tr>
<td>( r_s )</td>
<td>1 ( R_\ast )</td>
</tr>
<tr>
<td>( C/O )</td>
<td>0.75</td>
</tr>
<tr>
<td>( \dot{M} )</td>
<td>(0.4 - 3) ( \times 10^{-5} ) ( M_\odot/\text{yr} )</td>
</tr>
<tr>
<td>( \Psi )</td>
<td>1.9 ( \times 10^{-2} )</td>
</tr>
</tbody>
</table>
Gas-phase chemistry

Molecular detections in inner oxygen-rich AGB winds:

\( \text{H}_2\text{O}, \text{OH, SiO, SiS, NaCl, CO, CO}_2, \text{HCN, CS, SO, SO}_2, \text{NH}_3 \)

\( \text{PN, PO} \)  

Chemical network contains termolecular & bimolecular (neutral-neutral, collisional fragmentation, radiative association) processes – no ions

<table>
<thead>
<tr>
<th>Reaction type</th>
<th>Reaction formulation</th>
<th>Gas conditions</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Unimolecular</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Thermal decomposition</td>
<td>( \text{AB} \rightarrow \text{A} + \text{B} )</td>
<td>High T</td>
</tr>
<tr>
<td><strong>Bimolecular</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Neutral-exchange</td>
<td>( \text{AB + C} \rightarrow \text{A + CB} )</td>
<td>T dependent</td>
</tr>
<tr>
<td>Collisional dissociation</td>
<td>( \text{AB + M} \rightarrow \text{A + B + M} )</td>
<td>High T</td>
</tr>
<tr>
<td>Radiative association</td>
<td>( \text{A + B} \rightarrow \text{AB} + \gamma )</td>
<td>T independent</td>
</tr>
<tr>
<td><strong>Termolecular</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Termolecular formation</td>
<td>( \text{A + B + M} \rightarrow \text{AB + M} )</td>
<td>(Very) high n</td>
</tr>
</tbody>
</table>

17 elements  
105 molecules  
426 reactions  

GOAL: Reproduce these molecules in the observed amounts
Chemical network

Bimolecular reaction: \( A + B \rightarrow C + D \)

Change in number density of species \( C \):

\[
\frac{dn(C)}{dt} = k_{AB} n(A)n(B)
\]

\[
k_{AB} = \alpha \left( \frac{T}{298 \text{ K}} \right)^\beta \exp \left( \frac{-E_a}{RT} \right)
\]

Set of reactions: Arrhenius reaction rate

\[
\frac{dn_i}{dt} = \sum_{j,k} k_{jk} n_j n_k + \sum_{j,k} k_{jkM} n_j n_k n_M - n_i \sum_l k_{il} n_l - n_i \sum_n k_n
\]

→ set of stiff, coupled, non-linear ordinary differential equations (ODEs)

→ ODEs subject to varying temperature and densities
Cluster nucleation routes

Chemical network involves formation pathways to dimers of alumina (Al$_2$O$_3$) & forsterite (Mg$_2$SiO$_4$), enstatite (MgSiO$_3$) of metal oxides (SiO, MgO, FeO, TiO), and pure metal clusters (Fe, Al, Si)

- Structure determination by a semi-classical Monte-Carlo-based candidate search & subsequent quantum Density Functional Theory (DFT) calculations
- DFT analysis yields thermochemical properties, which indicate trends for reaction mechanisms and kinetics

$\Delta G = \Delta H - T\Delta S$

Energetically favoured alumina tetramers $\text{Al}_8\text{O}_{12}$
Cluster nucleation routes

Silicates: forsterite dimers $\text{Mg}_4\text{Si}_2\text{O}_8$

- SiO dimerisation too slow to start silicate nucleation
- Nucleation proceeds via HSiO, $\text{H}_2\text{Si}_2\text{O}_2$ & $\text{H}_2\text{Si}_2\text{O}_3$ formation
- Growth via successive oxidation & Mg inclusion steps
- Efficient mechanism to synthesise silicate dimers (enstatite and forsterite) between $\sim 4 \, R_*$ and $6 \, R_*$
Dust grain condensation

Formalism based on Brownian thermal motion, which accounts for the scattering, fragmentation, and coagulation of the grains \( \text{Plane 2013, Sarangi & Cherchneff 2014} \)

→ Grains size distributions are derived for silicates of forsterite and enstatite stoichiometry, and alumina.

→ Grains are assumed to be spherical, volume conserving and stable to (stellar) radiation

Timescales for dust condensation?
Consider from hydro models \( \text{Bowen 1988, Nowotny 2010} \)

Dust grains keep growing over several pulsation periods, whereas gas phase molecules reform within one period.

• Drift velocities at \( r > 3 \, R_* \) for silicates – 1.5 kms\(^{-1}\) correspond to two pulsations to cover 0.5 \( R_* \).
Results: Molecules in IK Tau

CO, H$_2$O, SiO, SiS, HCl, AIOH & PN form close to the star as soon as gas relaxes and cools down.

Gobrecht 2015 submitted

Some molecules are more shock chemistry-dependent. C-bearing species form from CO breaking by shocks SO, HCN, CS, CO$_2$
Results: Molecules in IK Tau

- Modelled abundances for 12 molecules at 6 R.* agree well with observations
- Validate shock chemistry scenario → strong impact of shocks on the gas and solid phases of the inner wind
- Discrepancy for SO$_2$

Our parent species include

CO, H$_2$O, SiO, SiS, PN, SO, HCN, CS, CO$_2$, AlOH, TiO, HCl & NaCl

Gobrecht 2015 submitted
Results: Dust clusters in IK Tau

Alumina dimers $\text{Al}_4\text{O}_6$:

Form at 1 $R_*$ when $T_{\text{gas}} < 2000$ K

Abundance of dimers on the low side

Other formation channels, which deplete $\text{AlOH}$?
Results: Dust clusters in IK Tau

Silicates: forsterite dimers $\text{Mg}_4\text{Si}_2\text{O}_8$

Start forming at 3.5 $R_*$ from HSiO dimerisation.
Grain size distributions: alumina

Large grains > 0.02 μm are already formed at 1, because gas densities are high in the postshock gas.
- Forsterite grains grow to larger sizes with increasing number of pulsations and radius.
- Dust/gas mass ratio after 8 R* agrees with observations.
- Grain size peaks at 0.02 μm, which is a bit low (from obs. a = 0.1 μm).
A factor x10 in gas density results in grain size distributions peaking at ~ 0.1 μm \(\rightarrow\) inhomogeneous wind will help!
Semiregular variables

Regularity classes (Mira, Sra, Srb and Irregular) are rather loosely defined in GCVS

- **Mira**: $M_v > 2.5$ mag, $P > 100$ d
- **Sra**: Mixture of Miras and Srbs
- **Srb**: $T_\ast > 3200$ K, $P < 150$ d

Stellar parameters of SRVs compared to Mira variables:

- $T_\ast$, $M_\ast$ are higher
- $P$, $R_\ast$, $C/O$, $v_{\text{term}}$, $\dot{M}$ are lower

=> interpreted as stars on the early AGB
Results for W Hydrae (SRa)

Alumina grains form, silicate clusters form, but at too low gas density to efficiently condense.
Results: S-type star

Molecular abundances vs. Radius for a 20 km/s shock and parameters for W Aquilae

Comparison of modelled abundances with the most recent Herschel/HIFI and previous observations

Danilovich 2014
Alumina and forsterite grains form in quantity and large sizes, despite the comparable high C/O = 0.95. Observations predict a mass loss rate of $3 \cdot 10^{-6} \text{ M}_{\odot}/\text{yr}$ and a dust-to-gas mass ratio of $5 \cdot 10^{-3}$. This is consistent with our dust-to-gas mass ratio at $8 \text{ R}_*$:

$\Psi = 4 \cdot 10^{-3}$ for a 20 km/s shock and $\Psi = 6 \cdot 10^{-3}$ for a 32 km/s shock.
Miras in the SMC

Alumina dust:
\[ \Psi = 1.3 \cdot 10^{-8} \]
\[ A_{\text{grain}} = 13 \, \text{Å} \]

Forsterite dust:
\[ \Psi = 3.1 \cdot 10^{-4} \]
\[ A_{\text{grain}} = 75 \, \text{Å} \]

[Graphs showing abundance and grain radius distributions]
Miras in the LMC

Alumina dust:
Ψ = 3.2 \cdot 10^{-6}
A_{\text{grain}} = 115 \text{ Å}

Forsterite dust:
Ψ = 1.1 \cdot 10^{-3}
A_{\text{grain}} = 110 \text{ Å}

Z = 0.008
D = 50 \text{ kpc}
Conclusions

• Pulsation models of the inner wind of Mira stars well explain observed molecular abundances of H$_2$O, OH, SiO, SiS, CO, CO$_2$, HCN, CS, SO, PN and HCl.

• NH$_3$, SO$_2$ and PO cannot be reproduced by the models. Observations indicate that these species
  - are located outside the inner envelope or
  - synthesized by processes not considered here (photochemistry, grain surface reaction).

• Alumina grains (> 0.1 µm) form close to the star at r ≤ 1.5 R$_*$. 

• Silicate (forsterite) grains form between 4 R$_*$ and 6 R$_*$ from a new nucleation route involving HSiO

→ Consistent with recent MIDI/VLT observations

Karovicova 2013
Conclusions

Semi-regular (SRV) model: Molecular abundances agree with observations (CO, SiO, HCN). Alumina dust forms, but silicates can hardly be synthesized, owing to low densities.

S-type star model: Models predict large amounts of alumina and silicate dust. Modelled abundances (in particular SiO and H$_2$O) agree with observations before the onset of forsterite formation.

Low metallicity model: Smaller amounts of clusters and dust are derived, owing to the lower availability of heavy elements.

For the first time, detailed non-equilibrium chemical models accounting for - gas phase,
- cluster nucleation, and
- dust condensation,
are set up for the inner winds of AGB stars (O-rich Miras, semi-regular, S-type, and Miras in the SMC/LMC) and explains the prevalent molecules and dust condensates.
Questions

Any questions?
Suggestions for improvement?
Looking for experts in Hydrodynamics!